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DEPARTMENT OF INORGANIC CHEMISTRY

Crystal Structure Determination of Synthetic Tellurate (IV) Compounds

Göran B. Johansson

1978

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CRYSTAL STRUCTURE DETERMINATION OF SYNTHETIC TELLURATE(IV) COMPOUNDS

Göran B. Johansson

AKADEMISK AVHANDLING

som med tillstånd av kemiska sektionsnämnden vid Göteborgs Universitet framlägges till offentlig granskning för avläggande av filosofie doktorsexamen i oorganisk kemi den 28 april 1978 kl 1015 i föreläsningssal KA, Kemihuset, Chalmers Tekniska Högskola, Göteborg.

GÖTEBORG 1978

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CRYSTAL STRUCTURE DETERMINATION OF SYNTHETIC TELLURATE(IV) COMPOUNDS

Göran B. Johansson

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This thesis is a resumé of work presented in detail in the following papers:

I The Crystal Structure of $Al_2(OH)_2TeO_3SO_4$.
Göran B. Johansson and Oliver Lindqvist.
Acta Cryst. (1976). B32, 407 - 411.

II Ditellurium(IV) Trioxosulphate.
Göran B. Johansson and Oliver Lindqvist.
Acta Cryst. (1976). B32, 2720 - 2722.

III The Crystal Structure of Amminecopper(II) Tellurate(IV) Monohydrate, $Cu(NH_3)TeO_3 \cdot H_2O$.
Göran B. Johansson and Oliver Lindqvist.
Acta Cryst. (1977). B33, 2418 - 2421.

IV The Crystal Structure of Dipotassium Tellurate(IV) Trihydrate, $K_2TeO_3 \cdot 3H_2O$.
Göran B. Johansson and Oliver Lindqvist.
Acta Cryst. (1978). In press.

V Diammonium Ditellurium(IV) Pentaoxide Dihydrate.

Göran B. Johansson.

Acta Cryst. (1978). In press.

In addition, the construction of equipment for hydrothermal syntheses at pressures up to 4000 atm. and temperatures up to 600 ^{o}C is described.

INTRODUCTION

Tellurium (from Lat. tellus) was first discovered in 1782 by the Austrian F.J. Mueller von Reichenstein in a gold-mine district of Transylvania (Cooper, 1971). The mineral found was described both as white and as gray-gold, and it was generally considered to be an alloy of bismuth and antimony. Mueller von Reichenstein observed, however, that it did not show any characteristic properties of these two metals, and supposed it to be a new metal, which he called metallum problematicum or aurum paradoxum. The Swedish chemist Torbern Bergmann also discovered this new metal, but never gave it a name. Some years later another Austrian chemist, M.H. Klaproth, showed that the metal from the mineral had unique properties, and he gave it the name Tellurium.

Since then, several minerals containing tellurium have been examined, and several tellurium compounds have been synthesized. The first crystallographic structure determination of a tellurate(IV) was undertaken in 1949 on the mineral Paratellurite, α-TeO_2, by Stěhlik and Bálák. The crystal structures of other minerals like Teineite, $CuTeO_3 \cdot 2H_2O$, Zemannite, $[(Zn,Fe)_2(TeO_3)_3]Na_xH_{2-x} \cdot yH_2O$, Denningite, $(Mn,Ca,Zn)[Te_2O_5]$, Mackayite, $Fe(OH)[Te_2O_5]$, Carlfriesite, $CaTe_3O_8$ and Mroesite, $CaTeO_2(CO_3)$ have been determined by Josef Zemann and his coworkers (cf. Zemann, 1971).

Previous crystallographic investigations of synthetic tellurates(IV) have been performed by Galy (1971), Moret (1972), Lindqvist (1973), and other workers.

Table 1. A summary of results from syntheses of tellurates(IV) with different cations

Formula	Synthesis method	Cell dimensions a (Å)	b (Å)	c (Å)	Crystal shape
		α (°)	β (°)	γ (°)	
$Al_2(OH)_2TeO_3SO_4$	H	7.013(2)	9.539(4)	4.880(2)	Colourless plates
			92.65(3)		Monoclinic
$Te_2O_3SO_4$	H	4.654(1)	6.936(1)	8.879(2)	Colourless plates
					Orthorombic
$Cu(NH_3)TeO_3 \cdot H_2O$	H	12.988(4)	7.333(1)	10.022(3)	Blue plates
			97.18(3)		Monoclinic
$K_2TeO_3 \cdot 3H_2O$	M	8.930(3)	6.973(3)	12.481(3)	Colourless parallel-epipeds
					Orthorhombic
$(NH_4)_2Te_2O_5 \cdot 2H_2O$	H	10.357(2)	11.000(2)	8.178(2)	Colourless prisms
			93.23(1)		Monoclinic
Na_2TeO_3	M				Colourless rods
$Na_2TeO_3 \cdot 5H_2O$	Aq	6.182	6.182	13.560	Colourless hexagonal plates
		90.0	90.0	120.0	
$(NH_4)_2Te_4O_9 \cdot 4H_2O$	Aq	10.775(6)	10.775(6)	13.481(9)	Colourless hexagonal plates
		90.0	90.0	120.0	
Ag_2TeO_3(I)	H	9.682	3.692	7.406	Yellow plates
		120.97	80.32	95.57	Triclinic
Ag_2TeO_3(II)	H	9.075(2)	9.269(3)	13.662(4)	Black plates
			91.75(2)		Monoclinic
K_2TeO_3	Aq				Colourless rods
$K_2Te_2O_5$	Aq				Colourless rods
$Te_2O_4 \cdot HClO_4$	H	8.940(5)	7.310(4)	9.043(7)	Colourless rods
		99.09(5)	91.21(6)	54.86(3)	

A = Aqueous solution

H = Hydrothermal syntheses

M = Obtained from melt

conditions as used at the Department of Inorganic Chemistry, University of Montpellier, France (Moret, 1972).

0.21 g of $Al_2(SO_4)_3 \cdot 18H_2O$ and 0.2 g of TeO_2 were mixed and placed in a small gold tube and 0.8 ml distilled water was added, together with a small amount of sulphuric acid. The gold tube was sealed and placed in an autocalve of the Bridgeman type. The bomb was filled with sufficient water to achieve a pressure of about 2000 atm., when sealed and heated to a temperature of 650 °C. After 24 hours the heating was stopped and the bomb, after being allowed to cool, was opened. Thin colourless plates of $Al_2(OH)_2TeO_3SO_4$ were obtained in an acidic mother liquor.

$Te_2O_3SO_4$

The synthesis of $Te_2O_3SO_4$ has been discussed by Hubková, Loub and Syneček (1966). The preparation of crystals for this investigation was carried out in two different ways starting either from $Te(OH)_6$ or from TeO_2.

1) 0.63 ml concentrated sulphuric acid and 1.25 g orthotelluric acid were placed in a pyrex tube of volume 2.5 ml. The glass tube was sealed by melting and then placed in a furnace for 10 hours at a temperature of 370 °C. The tube was opened with a special knife because of the risk for explosion due to excess oxygen liberated during the process.

2) 0.9 g TeO_2, 0.8 ml sulphuric acid and 0.38 ml distilled water were placed in another pyrex tube and held at a temperature of 400 °C for 12 hours.

White rods of $Te_2O_3SO_4$ are formed in both cases.

$Cu(NH_3)TeO_3 \cdot H_2O$

For the preparation of $Cu(NH_3)TeO_3 \cdot H_2O$ it was necessary to use $Cu(OH)_2$ and not CuO as stated in Paper III. Copper(II) hydroxide had to be prepared, because it was not possible to purchase it (Brauer, 1962). 25 ml concentrated $NH_3(aq)$ was added to 0.3 g TeO_2 and 0.2 g $Cu(OH)_2$ and the mixture was poured into a pyrex glass tube, which was sealed and heated to a temperature of 300 °C for 24 hours in an autoclave. Blue crystals and a Mediterranean blue liquid were obtained. These crystals were unstable in air and are now under investigation. The liquid was poured into a glass vessel and then into a desiccator with potassium hydroxide as drying medium (cf. Fig. 1). After two weeks, dark blue plates of $Cu(NH_3)TeO_3 \cdot H_2O$ appeared, which are stable in air.

$K_2TeO_3 \cdot 3H_2O$

Crystals of $K_2TeO_3 \cdot 3H_2O$ were prepared by fusing an equimolar mixture of potassium carbonate and tellurium dioxide in a platinum crucible. The mixture fused readily, carbon dioxide being evolved. In order to prevent oxidation, the air in the crucible was displaced by a stream of carbon dioxide from a cylinder. On cooling, a white crystalline mass was obtained, which was deliquescent, and extremely soluble in water. It was possible to isolate single crystals in dry air and mount them in glass capillaries. $K_2TeO_3 \cdot 3H_2O$ crystallizes as colourless parallelepipeds. The water content in the crystals originates from air humidity.

$(NH_4)_2 Te_2O_5 \cdot 2H_2O$

Crystals of $(NH_4)_2Te_2O_5 \cdot 2H_2O$ were prepared by adding an excess of

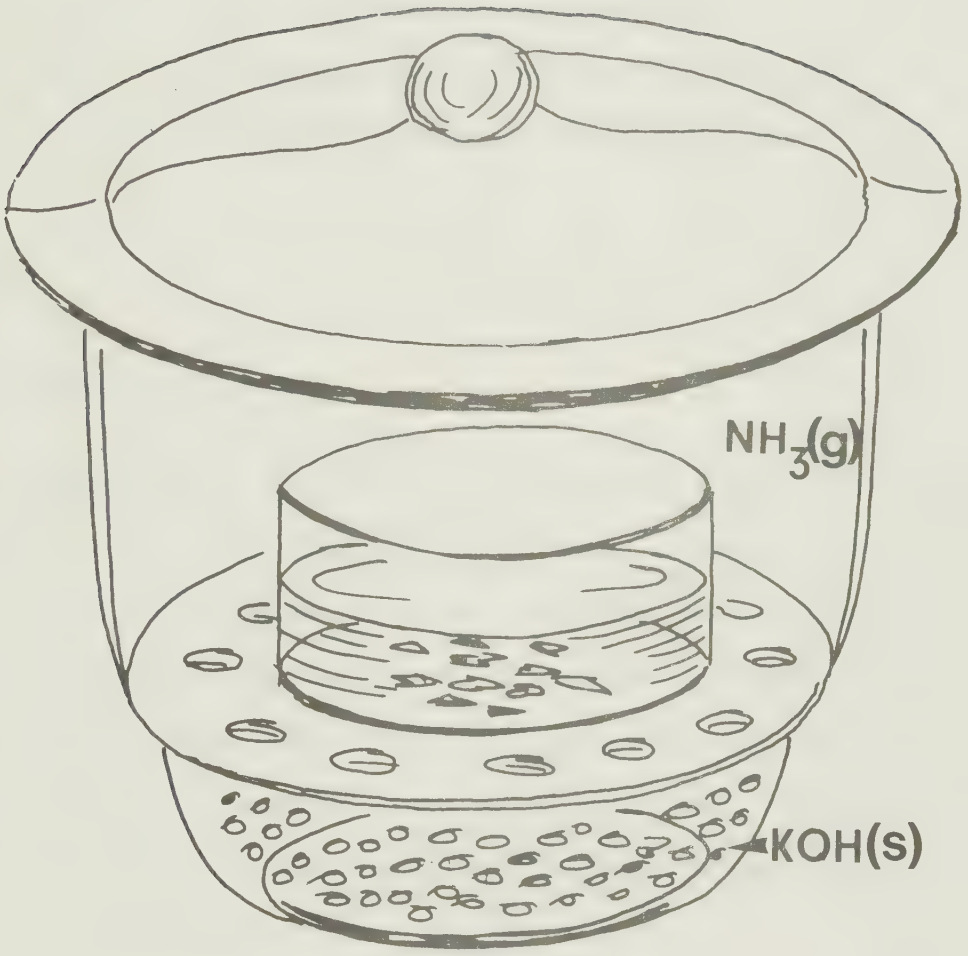

Fig. 1. The crystallization of $Cu(NH_3)TeO_3 \cdot H_2O$ and of $(NH_4)_2Te_2O_5 \cdot 2H_2O$, was performed in NH_3 atmosphere.

concentrated ammonia (about 200 ml) to 20 g tellurium dioxide. The mixture was heated to 50 - 100 °C for 12 to 48 hours in different attempts. The solution was then filtered at room temperature and allowed to crystallize in a desiccator containing solid potassium hydroxide (cf. Fig. 1). After a week prismatic crystals appeared. These were very unstable in air so it was necessary to work in a glove-box containing ammonia atmosphere (cf. Fig. 2).

HYDROTHERMAL SYNTHESES

Basic description

Hydrothermal synthesis of crystalline samples comprises the heating of solid material with water under pressure up to temperatures over the boiling point of water and often to temperatures over the critical point for water. The pressure, temperature and density at the critical point for water are: 217 atm, 374 °C and 0.32 g/ml. The syntheses take place in an autoclave, the upper limit for the hydrothermal pressure - and temperature area being set by the autoclave material.

Geologists and mineralogists were the first to use the hydrothermal synthesis method to produce, synthetically, naturally occurring minerals, e.g. silicates, carbonates, oxides and hydroxides.

It is very difficult to have complete knowledge of the different reactions that take place in an autoclave under hydrothermal conditions, and usually it is only possible to give an over-all reaction formula.

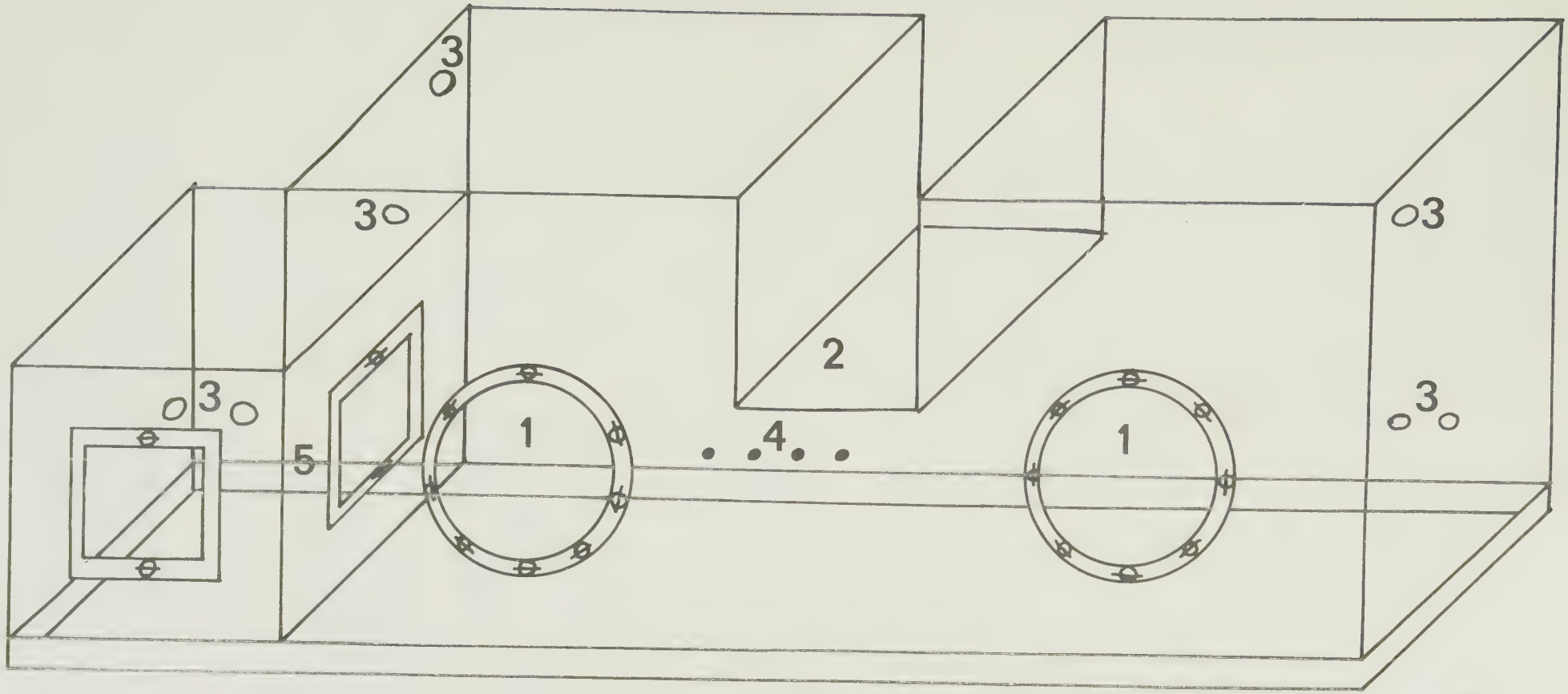

Fig. 2. The glove-box used (plexi-glass) for work in ammonia atmosphere. 1) Glove-holders. 2) Microscope can be inserted here. 3) Gas in- and outlets. 4) Electrical contacts. 5) Sluice.

Before determining the coefficient of filling of the autoclave, it is necessary to decide at what pressure and temperature the hydrothermal synthesis reaction will take place. The coefficient of filling is then determined according to Kennedy (1950 and 1958). The Figures 3 and 4 show pressure as a function of the temperature, and permit determination of the coefficient of filling. As an example, if a hydrothermal synthesis occurs at 1050 atm. and 400 ^{o}C, the coefficient of filling is 0.70 of the volume of the autoclave. This means that if the autoclave has a volume of 50 ml and if the sealed reaction tube of glass or gold has an exterior volume of 10 ml, then the autoclave should be filled with 28 ml water. The same filling coefficient should be used in the reaction tube to avoid deformation.

The density - temperature curve for water(l) $\rightleftarrows$ water(g) is given in Figure 5. For an initial degree of filling less than the critical (0.32) in a sealed vessel, the liquid - gas meniscus will fall as the temperature is raised and the liquid phase will be lost at the temperature shown in Figure 5 at which the initial degree of filling equals the vapor density. The temperature will be less than the critical temperature. The meniscus will neither fall nor rise in a vessel filled to the critical amount but will disappear at the critical temperature (Laudise, 1961). Similarly for a degree of filling greater than the critical, the meniscus will rise and the vessel will be filled with liquid water at a temperature below the critical temperature.

A great advantage of synthesizing crystals by the hydrothermal method, is that the crystals are formed at relatively low temperatures. It may therefore be assumed that crystals produced in this way have a

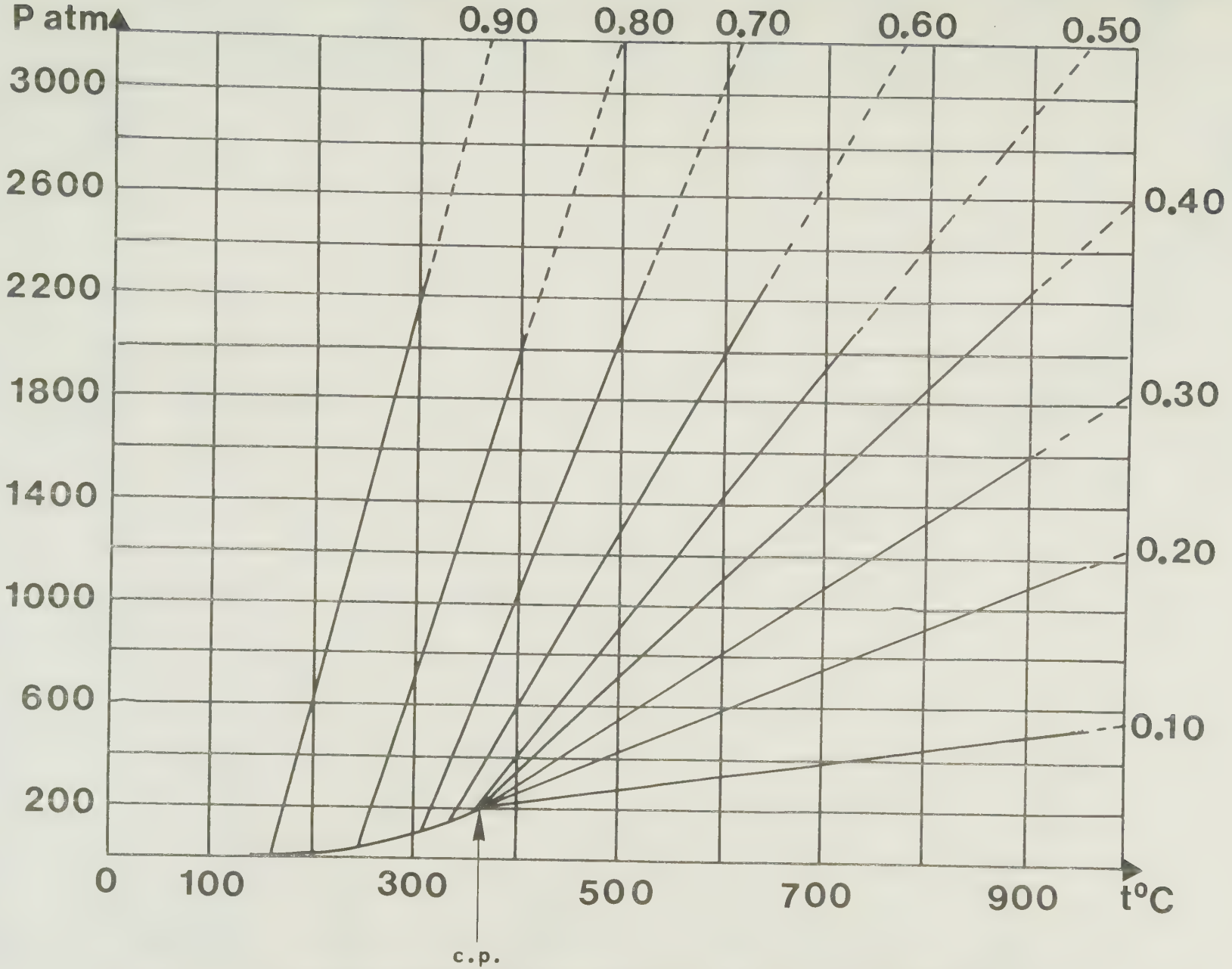

Fig. 3. The pressure-temperature curve with the filling coefficient (Kennedy, 1950). The critical point for water (217 atm. and 374 °C).

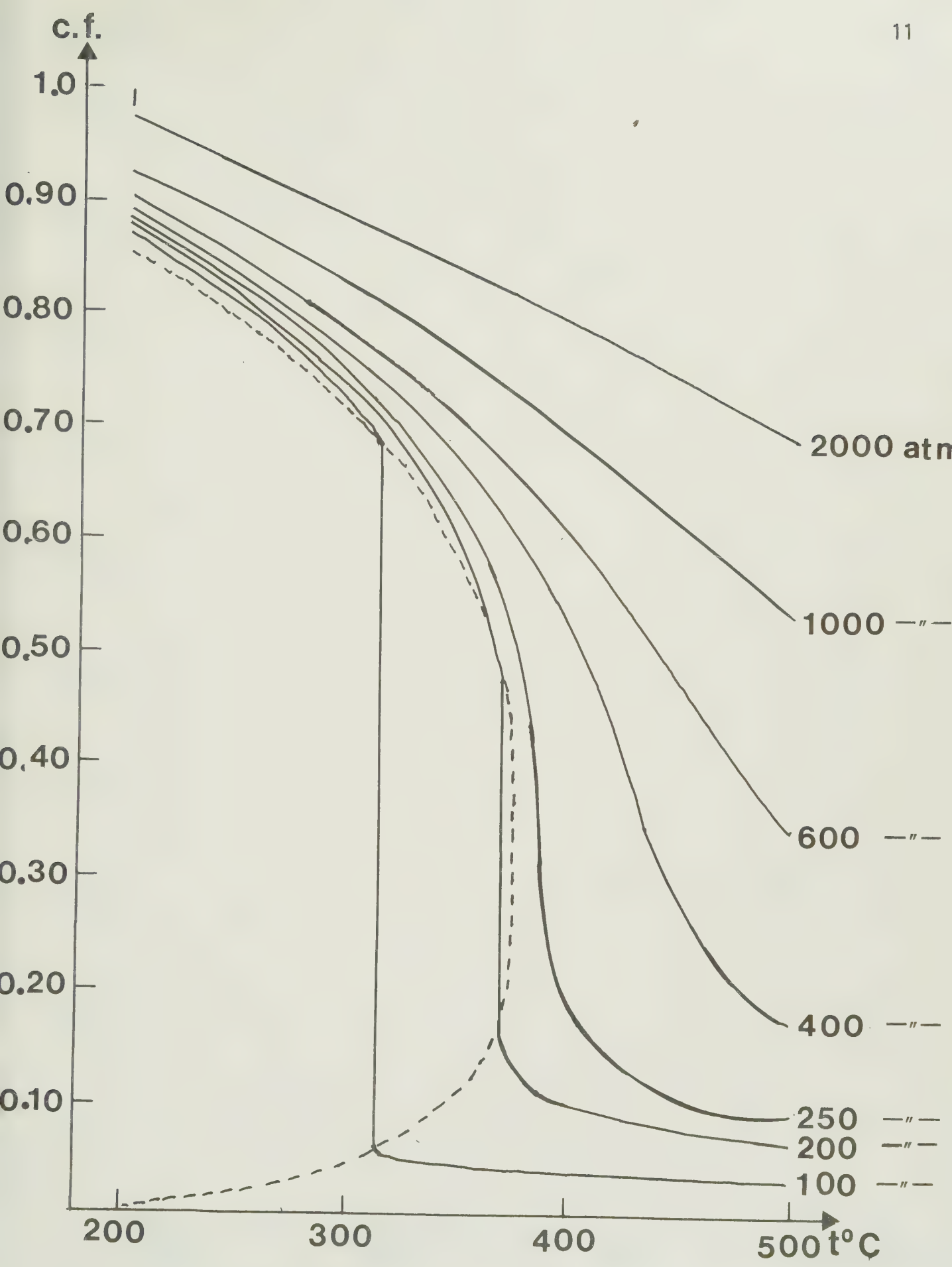

Fig. 4. The coefficient of filling in the autoclave (Kennedy, 1950 and 1958).

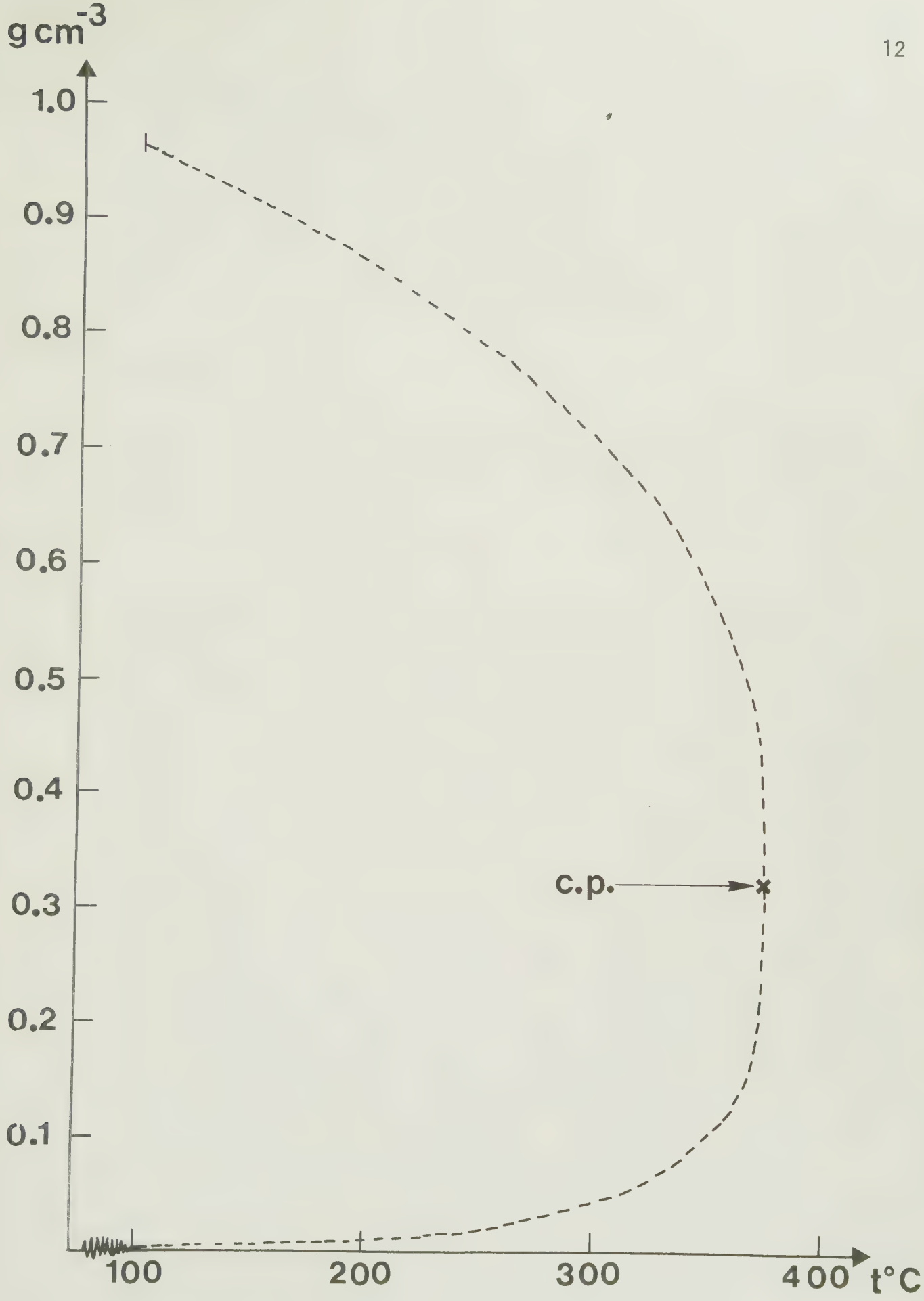

Fig. 5. The density-temperature curve for water(l) ⇄ water(g) (c.p. stands for the critical point for water; 374 °C,

higher degree of order than those crystals prepared from melts. Another advantage of hydrothermal syntheses is the possibility of obtaining metastable phases and compounds with elements in unusual oxidation states. These advantages outweigh the problems that always occur when working with hydrothermal syntheses.

Apparatus

The autoclaves used in Montpellier, France, for the synthesis of some of the compounds dealt with in this thesis have already been described (Moret, 1972).

Hydrothermal synthesis equipment has also been built up at this department. The construction details have been designed in cooperation with Dr. Sten Andersson, Lunds' University of Technology. The system (cf. Fig. 6) consists of two autoclaves made of an alloy of steel and nickel, known as Nimonic. This material is very flexible and therefore resists high pressure at high temperature. The autoclaves are connected to a high pressure pump *via* pipe-lines, specially made for pressures up to 10000 atm. The pump is used as a prepressure--giving apparatus up to 1000 atm., before the autoclaves are sunk into the furnaces. The furnaces used in this hydrothermal equipment have been constructed and built at this department. They consist of tube elements (Kanthal), isolation material (Fiberflax) and envelopes of aluminium (cf. Fig. 7). A manometer is coupled to each autoclave and holes have been drilled in the bottom of the autoclaves to facilitate measurement and regulation of the temperature by a thermocouple. There are valves between the autoclaves so that the pressures and temperatures in them can be varied independently.

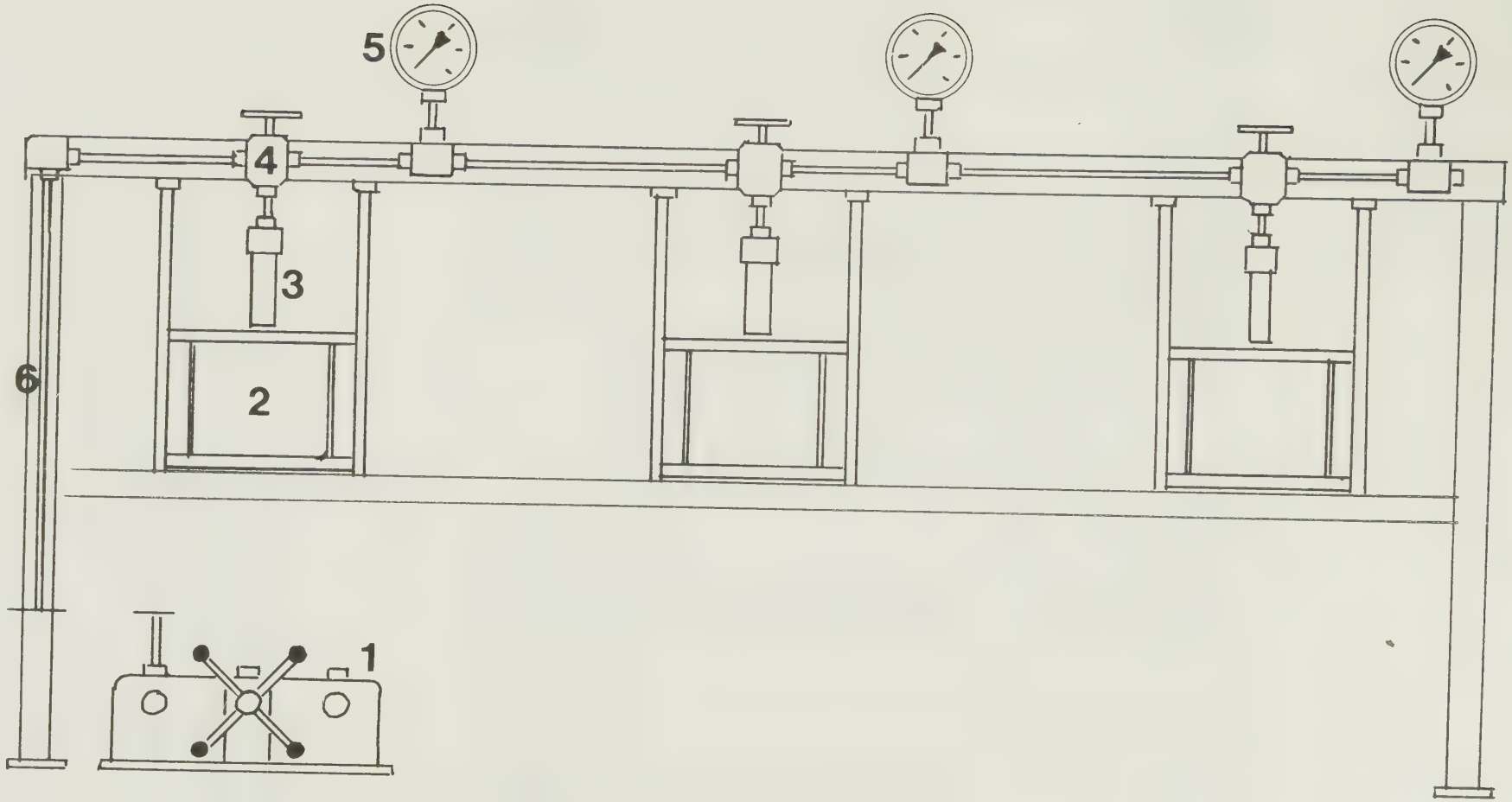

Fig. 6. The hydrothermal equipment. 1) Pump for giving a prepressure. 2) The furnace for heating. 3) The autoclave. 4) Valvet. 5) Manometer. 6) High-pressure pipe-line.

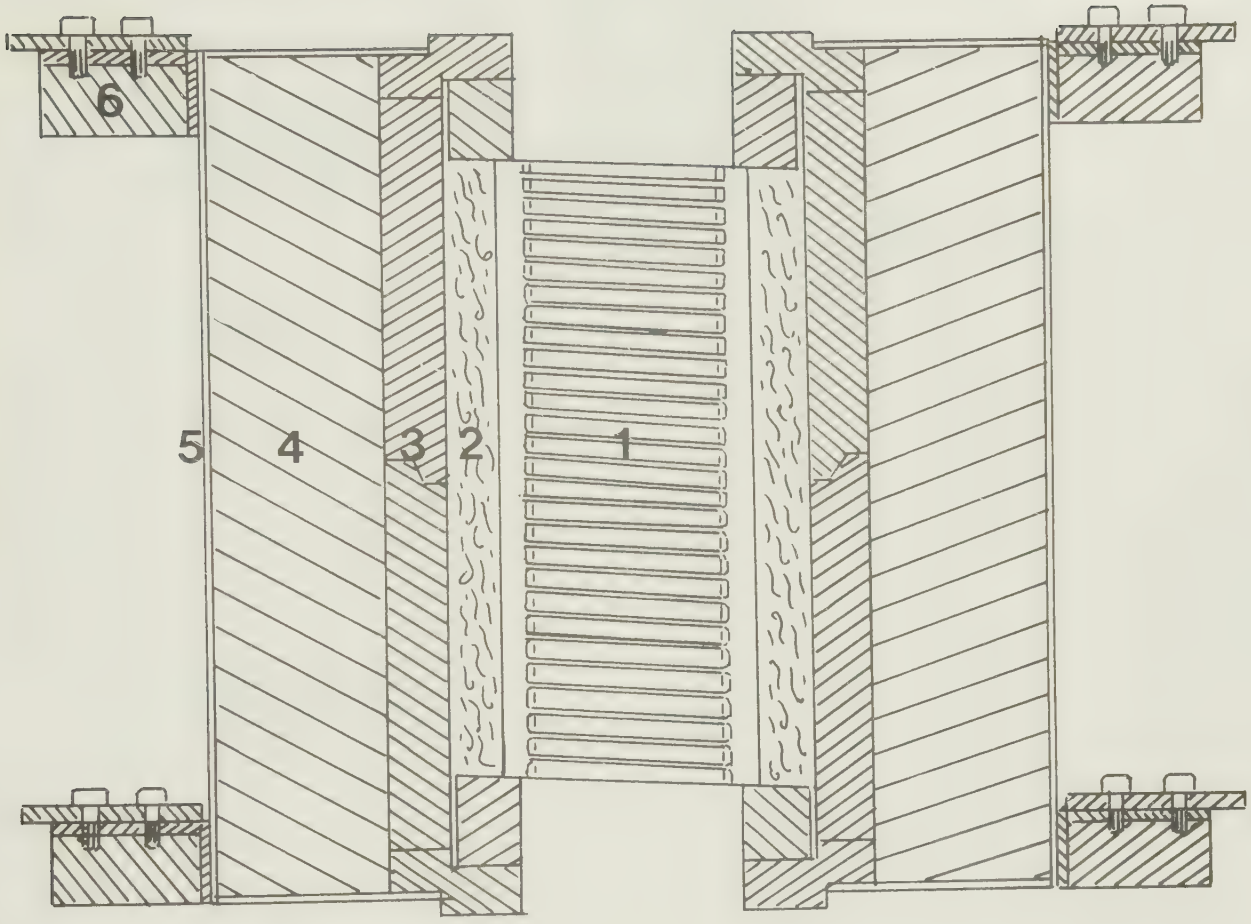

Fig. 7. An intersection of the furnace used. 1) The heating element. 2) and 4) Fiber isolation material. 3) Ceramic tube. 5) The envelope of aluminium. 6) The hanging arrangement.

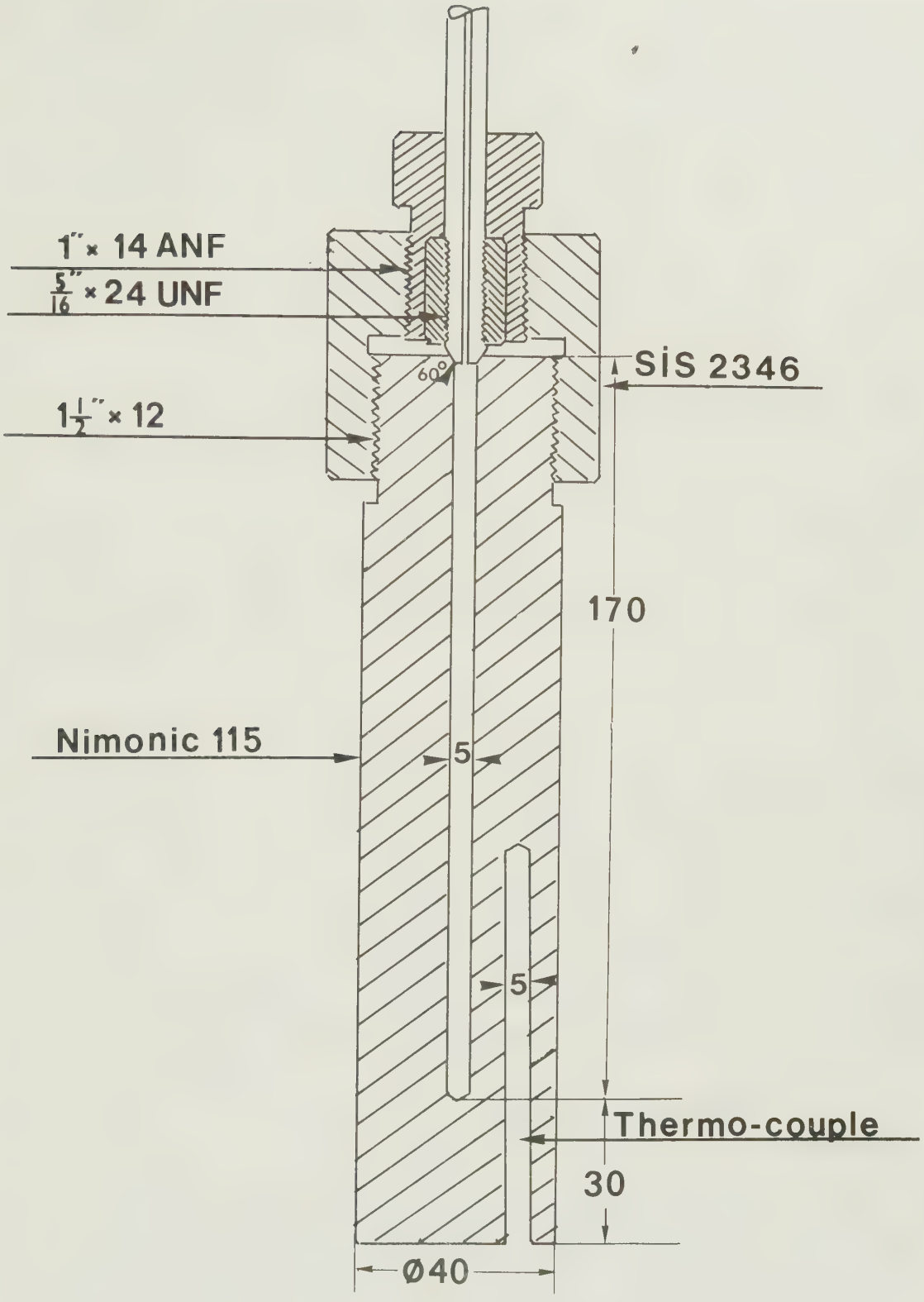

Fig. 8. A detailed drawing of the autoclave. The distances are given in mm.

Figure 6 shows the construction of the equipment and Figure 8 a detailed drawing of the autoclave. The upper limit for the system is 4000 atm. and 600 °C. The syntheses take place in sealed glass or gold tubes, which are placed in the autoclaves.

CRYSTALLOGRAPHIC METHODS AND PROGRAMS

Intensities for $Al_2(OH)_2TeO_3SO_4$, $Te_2O_3SO_4$ and $Cu(NH_3)TeO_3 \cdot H_2O$ were measured with a Philips PAILRED two-circle diffractometer, while data for $K_2TeO_3 \cdot 3H_2O$ and $(NH_4)_2Te_2O_5 \cdot 2H_2O$ were obtained with a four-circle Syntex $P2_1$ diffractometer. The radiation used was in all cases MoKα (λ = 0.71069 Å), monochromated with a graphite single crystal.

Preliminary cell dimensions and space groups were determined from Weissenberg films. For the first three structures mentioned above these values were used as starting values for the calculation of cell dimensions from Guinier powder photographs taken with KCl as an internal standard ($a = 6.2919_4$ Å at 20 °C, Hambling, 1953) using the program POWDER (Lindqvist and Wengelin, 1967). Cell dimensions are listed in Table 1.

A summary of single crystal data collection procedures used in the investigations is given in Table 2 and a summary of refinement results is given in Table 3.

Corrections for Lorentz and polarization effects were applied in the usual way. The data for all the structures, except $(NH_4)_2Te_2O_5 \cdot 2H_2O$, were corrected for absorption. Normally, absorption errors

Table 2. Data for intensity collection and for absorption corrections.

Compound	Data collection procedure	Radiation	Crystal dimensions (mm) (a x b x c)	Setting	No. of refl. (total)	Absorption correction	Extinction correction	μ_λ cm^{-1}	Gaussian grid (axbxc)	Transmission range
$Al_2(OH)_2TeO_3SO_4$	Philips PAILRED 2-circle diffr.	MoKα	0.011x0.058x0.148	[001]	1616	yes	yes	53.4	2x6x6	0.53 - 0.90
$Te_2O_3SO_4$	Philips PAILRED 2-circle diffr.	MoKα	0.0574x0.0858x0.0972	[100]	2325	yes	no	177.6	8x4x2	0.21 - 0.40
$Cu(NH_3)TeO_3 \cdot H_2O$	Philips PAILRED 2-circle diffr.	MoKα	0.0025x0.0260x0.0180	[010]	3418	yes	no	97.5	2x4x6	0.17 - 0.76
$K_2TeO_3 \cdot 3H_2O$	Syntex $P2_1$ 4-circle diffr.	MoKα	0.10x0.10x 0.30	A	2290	yes	yes	25.1	9x7x4	0.74 - 0.82
$(NH_4)_2Te_2O_5 \cdot 2H_2O$	Syntex $P2_1$ 4-circle diffr.	MoKα	0.10x0.09x0.19	A	3040	no	yes *	-	-	-

* Removal of reflections with severe extinction effects.

Table 3. Summary of refinement results. The R value is defined as $\Sigma||F_o| - |F_c||/\Sigma F_o$

Compound	Space group	Number of atoms in the asymm. unit	Number of parameters	Number of reflections per param.	Final R
$Al_2(OH)_2TeO_3SO_4$	$P2_1/m$	9	68	23	0.032
$Te_2O_3SO_4$	$P2_1nm$	7	51	21	0.047
$Cu(NH_3)TeO_3 \cdot H_2O$	C2/c	8	67	20	0.040
$K_2TeO_3 \cdot 3H_2O$	Pnma	7	50	17	0.036
$(NH_4)_2Te_2O_5 \cdot 2H_2O$	$P2_1/c$	11	100	24	0.031

affect the thermal parameters but have no influence on the atomic positions. The absorption corrections were generally not applied until the structure was known. For the three first structures (Papers I, II, III) the program DATAP2 (Coppens, Leiserowitz and Rabinovich, 1965) was used for absorption correction, while for $K_2TeO_3 \cdot 3H_2O$ a modification of DATAP2 due to Hamilton (1971), DATAPH was used. For $(NH_4)_2Te_2O_5 \cdot 2H_2O$ it was not possible to apply a correction for absorption since it was necessary to mount the crystal in a glass capillary filled with epoxy-glue, which covered the whole of the crystal.

For $Al_2(OH)_2TeO_3SO_4$ and $K_2TeO_3 \cdot 3H_2O$ a secondary extinction parameter was included in the least-squares refinement of the structural parameters, according to Coppens and Hamilton (1970). In the $Te_2O_3SO_4$ and $Cu(NH_3)TeO_3 \cdot H_2O$ investigations in which no correction was applied for extinction, it would appear that no severe omission has been made. Errors evidently due to extinction can be seen in $(NH_4)_2Te_2O_5 \cdot 2H_2O$, where some of the most strongly affected reflexions have been removed in the final cycles of least-squares refinement.

Patterson functions and successive electron density calculations were used to determine the atomic positions (program DRF; Zalkin, Berkeley). In the initial stages of the refinement a block-diagonal approximation was used (program BLOCK, Lindgren, 1977) while the final cycles were carried out with a full-matrix least-squares program (LINUS, Coppens and Hamilton, 1970). For $Te_2O_3SO_4$ and $(NH_4)_2Te_2O_5 \cdot 2H_2O$ full-matrix refinement was not employed.

Bond distances and angles have been calculated from the atomic

positions obtained in the least-squares refinement. The program used was DISTAN written by Zalkin, Berkeley.

As a confirmation of the correctness of the structures final difference syntheses were calculated.

DESCRIPTION OF THE STRUCTURES

Detailed descriptions of the structures are to be found in Papers I - V. In this section only the main structural arrangements will be summarized.

$Al_2(OH)_2TeO_3SO_4$

The structure of $Al_2(OH)_2TeO_3SO_4$ contains TeO_3 pyramids, SO_4 tetrahedra and dimeric Al - O octahedra, $Al_2(OH)_2O_8$. The Al - O octahedra share oxygen atoms to form infinite sheets (cf. Fig. 9). The layers are held together by van der Waals forces. In $Al_2(OH)_2TeO_3SO_4$ the tellurium(IV) coordination is three-fold pyramidal with Te - O distances of 1.902(3) - 1.939(4) Å. In addition there exist three longer contacts in the range 2.567(3) to 2.705(5) Å (cf. Fig. 10).

Aluminium has octahedral coordination and the two Al atoms are linked together by double hydroxide bridges. The coordination polyhedra also include oxygen atoms from three different TeO_3 groups and one sulphate ion. The Al - O bond distances appear to be in the normal range.

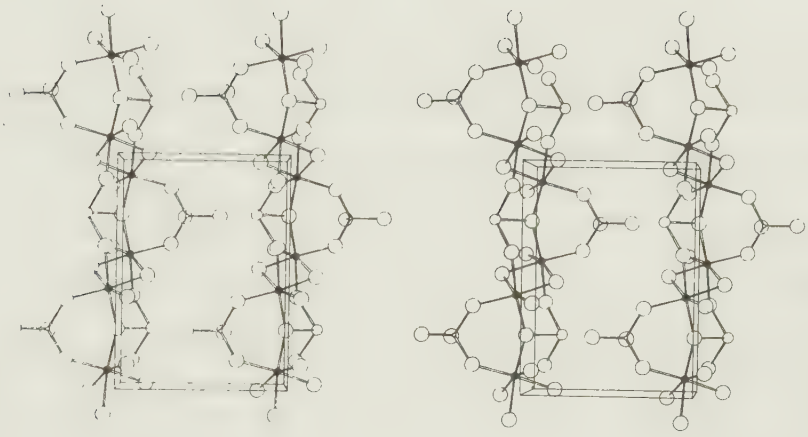

Fig. 9. A stereoscopic drawing of the structure along c showing the adjacent layers of $Al_2(OH)_2TeO_3SO_4$ (ORTEP; Johnson, 1965).

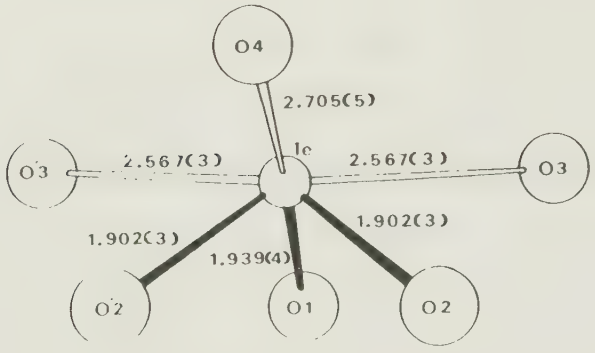

Fig. 10. The oxygen coordination of tellurium(IV) in $Al_2(OH)_2TeO_3SO_4$.

$Te_2O_3SO_4$

$Te_2O_3SO_4$ has a layer structure (cf. Fig. 11) in which the SO_4 tetrahedron is strongly connected to the layers by two Te - O bonds of 2.26(1) Å. The layers are held together by van der Waals forces.

The coordination of tellurium(IV) is intermediate between three- and four-fold. The four-fold coordination is usually described as a trigonal bipyramid in which the two shortest Te - O bonds are equatorial and the two other tellurium - oxygen bond distances have axial positions. The third equatorial position is occupied by the Te(IV) free electron pair. In this structure, however, three of these oxygen atoms lie in the same plane, while the fourth is situated perpendicular to this plane. In addition there are two weak Te - O interactions (2.63 and 2.84 Å, cf. Fig. 12).

$Cu(NH_3)TeO_3 \cdot H_2O$

The structure of $Cu(NH_3)TeO_3 \cdot H_2O$ is built up from TeO_3 pyramids bonded *via* oxygen bridges to three copper atoms. The copper(II) coordination is square planar with three corners of the square occupied by oxygen atoms from different TeO_3 groups and the fourth corner by an ammonia molecule (cf. Fig. 13). This arrangement results in infinite sheets separated by water of crystallization (cf. Fig. 14).

The tellurium atom has a threefold pyramidal coordination, with no "back-bonding" oxygen atoms closer than 2.950(7) Å. It may therefore be possible to describe the TeO_3 unit as being of ionic character.

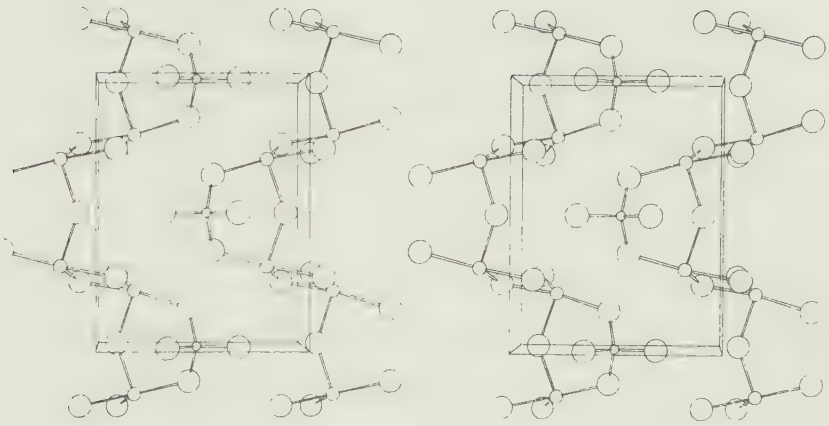

Fig. 11. A stereoscopic picture of $Te_2O_3SO_4$ projected along the c axis (ORTEP; Johnson, 1965).

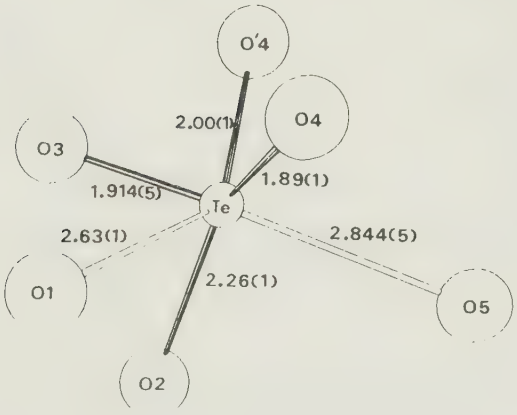

Fig. 12. The oxygen coordination around Te(IV) in $Te_2O_3SO_4$.

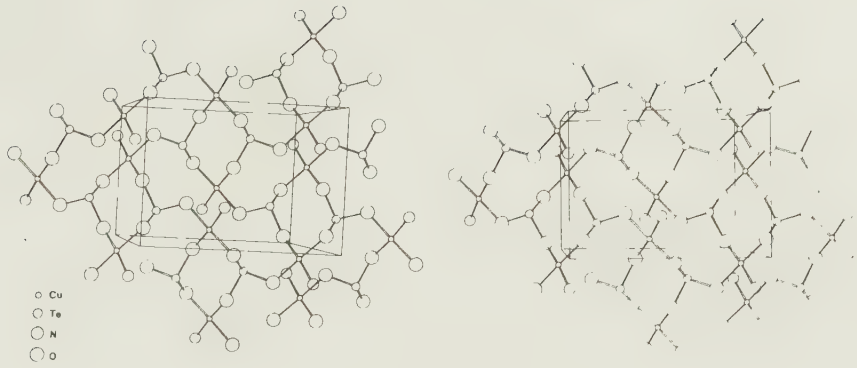

Fig. 13. A stereoscopic drawing of one $Cu(NH_3)TeO_3 \cdot H_2O$ layer (ORTEP; Johnson, 1965).

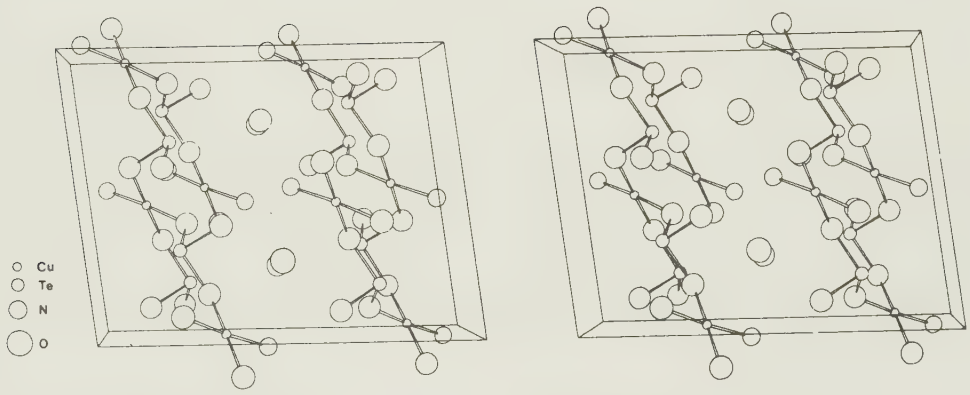

Fig. 14. The $Cu(NH_3)TeO_3 \cdot H_2O$ structure seen along the layers (ORTEP; Johnson, 1965).

$K_2TeO_3 \cdot 3H_2O$

The structure consists of TeO_3^{2-} ions, K^+ ions and water molecules, held together by electrostatic interactions and hydrogen bonds. Figure 15 shows a drawing of the structure.

The TeO_3^{2-} ion has a pyramidal configuration with the tellurium(IV) atom at the top of the pyramid. The tellurium - oxygen bond distances lie in the range 1.848(8) - 1.852(6) Å and the angles are 2 x 97.7(3)° and 102.4(3)°. The fourth closest oxygen atom is at 3.872(8) Å from tellurium.

The potassium ions both have six oxygen contacts at normal distances ranging from 2.684 Å to 2.983 Å for K(1) and 2.705 Å to 2.965 Å for K(2). K(1) has contacts only to water oxygen atoms, while K(2) has contacts both to water molecules and to TeO_3^{2-} ions.

$(NH_4)_2Te_2O_5 \cdot 2H_2O$

$(NH_4)_2Te_2O_5 \cdot 2H_2O$ contains infinite $[Te_2O_5]_n^{2n-}$ chains, in which two tellurium(IV) atoms from different Te_2O_5 groups share two oxygen atoms to form double oxygen bridges (cf. Fig. 16).

The two different Te atoms in the Te_2O_5 molecule share one oxygen atom, each Te being involved in three short and one long Te - O bond, i.e. three Te - O from 1.834(4) Å to 2.034(3) Å and a fourth of 2.218(3) Å for Te(1) and three Te - O from 1.840(3) Å to 1.971(4) Å and a fourth Te - O of 2.506(4) Å for Te(2) (cf. Fig. 17). It is possible to see the coordination around the two tellurium atoms as trigonal bipyramidal with two longer Te - O bonds in axial positions

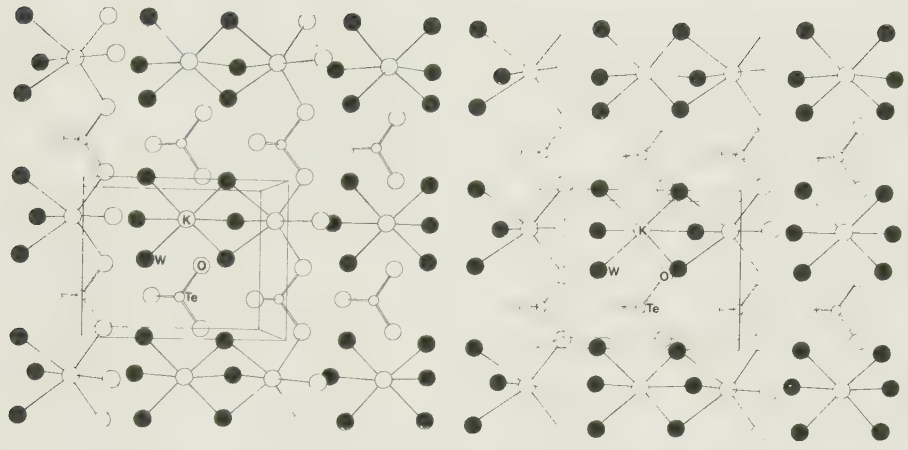

Fig. 15. A drawing of $K_2TeO_3 \cdot 3H_2O$ (ORTEP; Johnson, 1965).

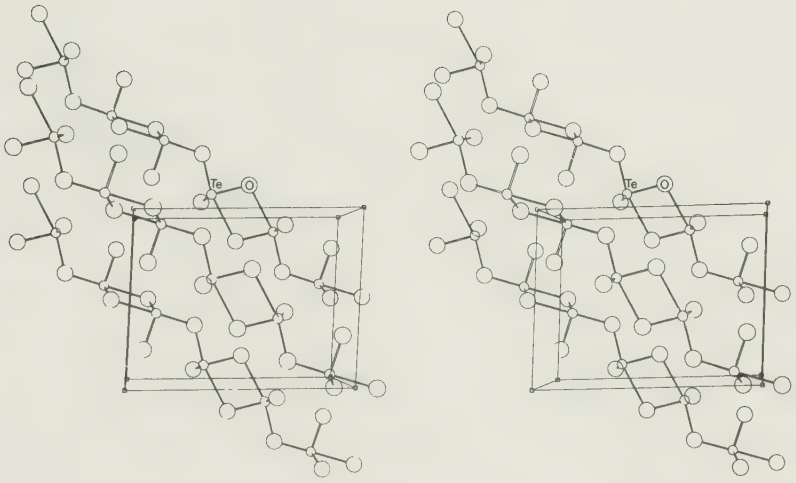

Fig. 16. A stereoscopic picture of the Te - O chains in $(NH_4)_2Te_2O_5 \cdot 2H_2O$ (ORTEP; Johnson, 1965).

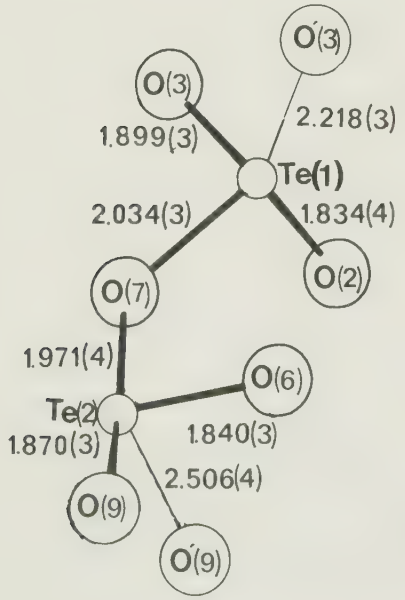

Fig. 17. The tellurium(IV)-oxygen coordination in $(NH_4)_2Te_2O_5 \cdot 2H_2O$ (ORTEP; Johnson, 1965).

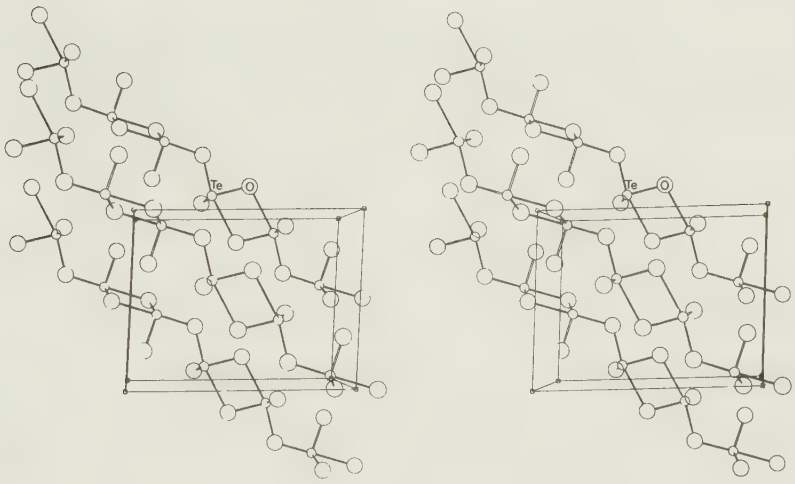

Fig. 16. A stereoscopic picture of the Te - O chains in $(NH_4)_2Te_2O_5 \cdot 2H_2O$ (ORTEP; Johnson, 1965).

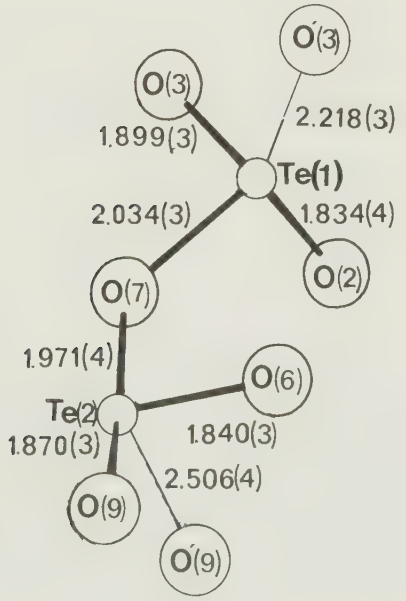

Fig. 17. The tellurium(IV)-oxygen coordination in $(NH_4)_2Te_2O_5 \cdot 2H_2O$ (ORTEP; Johnson, 1965).

and two shorter ones in equatorial positions, the third equatorial corner being occupied by the free $5s^2$ electron pair.

The ammonium ions and crystal water molecules are situated between the Te_2O_5 chains, the latter thus being connected by hydrogen bonds.

DISCUSSION

Previous descriptions of the structures of tellurates(IV) (Zemann, 1971; Lindqvist, 1973; Brown, 1974) have shown that tellurium(IV) can coordinate either three or four oxygen atoms, which is confirmed by the structures investigated in Papers I - V. It is not possible to describe the coordination around Te(IV) in terms of any one idealised polyhedron. In addition to the pure three-fold pyramidal and the four-fold trigonal bipyramidal configurations, there also exist intermediate forms, and, in addition, there may often be a fifth, and even a sixth, long contact to an oxygen atom.

In the following sections the details of different types of coordination occurring in tellurium(IV) oxocompounds will be discussed.

a) The TeO_3^{2-} ion

It is possible to precipitate tellurous acid, but the precipitate is unstable over 0 °C (Brauer, 1960)) and loses water to form tellurium dioxide. At 0 °C H_2TeO_3 is an amorphous white powder, which has prevented the determination of its structure. Compounds containing free TeO_3^{2-} ions seem to be rather unstable (Lindqvist and Johansson, 1976). The reason for this is that the Te(IV) free $5s^2$ electron pair

is probably very easy polarized. Pyramidal TeO_3^{2-} ions have only been found in a few compounds. In $BaTeO_3 \cdot 3H_2O$ (Rottersten-Nielsen, Grønbaek Hazell and Rasmussen, 1971) there are three oxygen atoms that coordinate in this way with bond distances very close to each other (cf. Table 4) and a mean Te - O of 1.855(4) Å and O - Te - O of 99.3(2)°. The fourth and fifth nearest oxygen atoms are 3.035(7) Å and 3.332(9) Å from the tellurium atom. $Cu(NH_3)TeO_3 \cdot H_2O$ (Paper III) can also be regarded as containing isolated TeO_3^{2-} ions, in which the mean of the three shortest Te - O bonds is 1.877(4) Å and the mean O - Te - O angle 96.1(1)°. The fourth, fifth and sixth nearest oxygen atoms are at 2.950(7) Å to 3.236(9) Å from the tellurium atom. A third compound exhibiting relatively pure Te(IV) three-fold coordination is Li_2TeO_3 (Folger, 1975), which has a layer structure where the lithium atom coordinates tetrahedrally to four different TeO_3 pyramids. The mean values of the three shortest Te - O distances and of O - Te - O angles are 1.88(2) Å and 99.8(5)°. The next longest Te - O distance is 3.19(2) Å which is similar to $BaTeO_3 \cdot H_2O$ (Nielsen et al, 1971). The TeO_3^{2-} ion in $CuTeO_3 \cdot 2H_2O$ (Effenberger, 1977) has a structure related to that in $Cu(NH_3)TeO_3 \cdot H_2O$ with an average Te - O distance of 1.87(1) Å and O - Te - O angle of 96.3(2)°. Distances and angles of ionic tellurates(IV) are compared in Table 4.

In all the examples mentioned above, there always exists a fourth and sometimes even a fifth and sixth oxygen atom that ought to have a slight effect on the three-fold coordination of tellurium(IV). The Te atom in these three-coordinated Te(IV) structures can be described as being sp^3 hybridized, the lone pair of electrons repelling the three bonding pairs (Gillespie and Nyholm, 1957) and thus causing the bond angles to decrease from the tetrahedral value of 109.47°.

Table 4. Distances (Å) and angles (°) for three-fold pyramidal Te - O coordination, with relatively isolated TeO_3^{2-} ions.

	$CuTeO_3 \cdot 2H_2O$[a]	$Cu(NH_3)TeO_3 \cdot H_2O$[b]	Li_2TeO_3[c]	$BaTeO_3 \cdot H_2O$[d]	$K_2TeO_3 \cdot 3H_2$
O_a:	1.86(1)	1.870(7)	1.93(2)	1.858(6)	1.848(8)
O_b:	1.86(1)	1.877(7)	1.85(2)	1.847(7)	1.852(6)
O_c:	1.88(1)	1.885(8)	1.87(2)	1.859(6)	1.852(6)
value*:	1.87(1)	1.877(4)	1.88(2)	1.855(4)	1.851(2)
O_d:	2.98(1)	2.950(7)	3.19(2)	3.035(7)	3.872(8)
Te - O_b:	96.6(5)	97.6(3)	98.9(9)	98.81(32)	97.7(3)
Te - O_c:	96.5(4)	96.1(4)	99.7(9)	96.49(28)	97.7(3)
Te - O_c:	95.8(4)	94.7(3)	100.7(9)	102.66(30)	102.4(4)
value*:	96.3(2)	96.1(1)	99.8(5)	99.32(18)	99.3(1)

a) Effenberger, 1977.

b) Paper III.

c) Folger, 1975.

d) Rottersten-Nielsen, Grønbaek Haxell and Rasmussen, 1971.

e) Paper IV.

* $$\sigma^2(\bar{b}) = \frac{1}{n-1} \frac{\Sigma(b_i-\bar{b})^2 \cdot \frac{1}{\sigma_i^2}}{\Sigma \frac{1}{\sigma_i^2}}, \qquad \text{(Hamilton, 1972)}$$

It is possible to regard the TeO_3^{2-} ion in $K_2TeO_3 \cdot 3H_2O$ as being unaffected by any "back-bonding" oxygen atom, due to the fact that the fourth nearest oxygen atom is situated 3.872(8) Å from the tellurium(IV) atom. The three Te - O bond lengths are: 1.848(8) Å, 1.852(6) Å x 2, giving an average value of 1.851(2) Å, while the O - Te - O angles are 97.7(3)° x 2 and 102.4(4)° with a mean value of 99.3(1)°. In $K_2TeO_3 \cdot 3H_2O$ the TeO_3^{2-} ion is essentially unpolarized which makes it possible to estimate the action radius of the $5s^2$ free electron pair (cf. Fig. 18). Galy, Meunier, Åström and Andersson (1975) have demonstrated that the Te(IV) free electron pair in condensed tellurates(IV) has a volume corresponding to that of an oxygen atom, i.e. the volume corresponds to a sphere of radius 1.25 Å. It has not, however, been possible to find any tellurate(IV) structure containing TeO_3-units in which a sphere of volume of 8.2 $Å^3$ could be accomodated. All condensed tellurates(IV) structures have the closest "back-bonding" atoms about 3 Å away, and the minimum distance between the Te(IV) atom and an O atom on the "backside" ought to be 2 x 1.25 + 1.40 Å = 3.90 Å. In $LiTeO_3$ (Folger, 1975) the relevant distance is 3.19 Å which gives a radius of 0.89 Å for the free electron pair, if the value 1.40 Å is used for the radius of the O atom (Shannon and Prewitt, 1969). In $K_2TeO_3 \cdot 3H_2O$ the "backside" Te - O distance is 3.87 Å and for the first time a sphere of radius 1.25 Å can be accomodated between the TeO_3 unit and the fourth distant oxygen atom. In fact the volume occupied by the free electron pair is probably greater than 8.2 $Å^3$ as the electron density is not spherical.

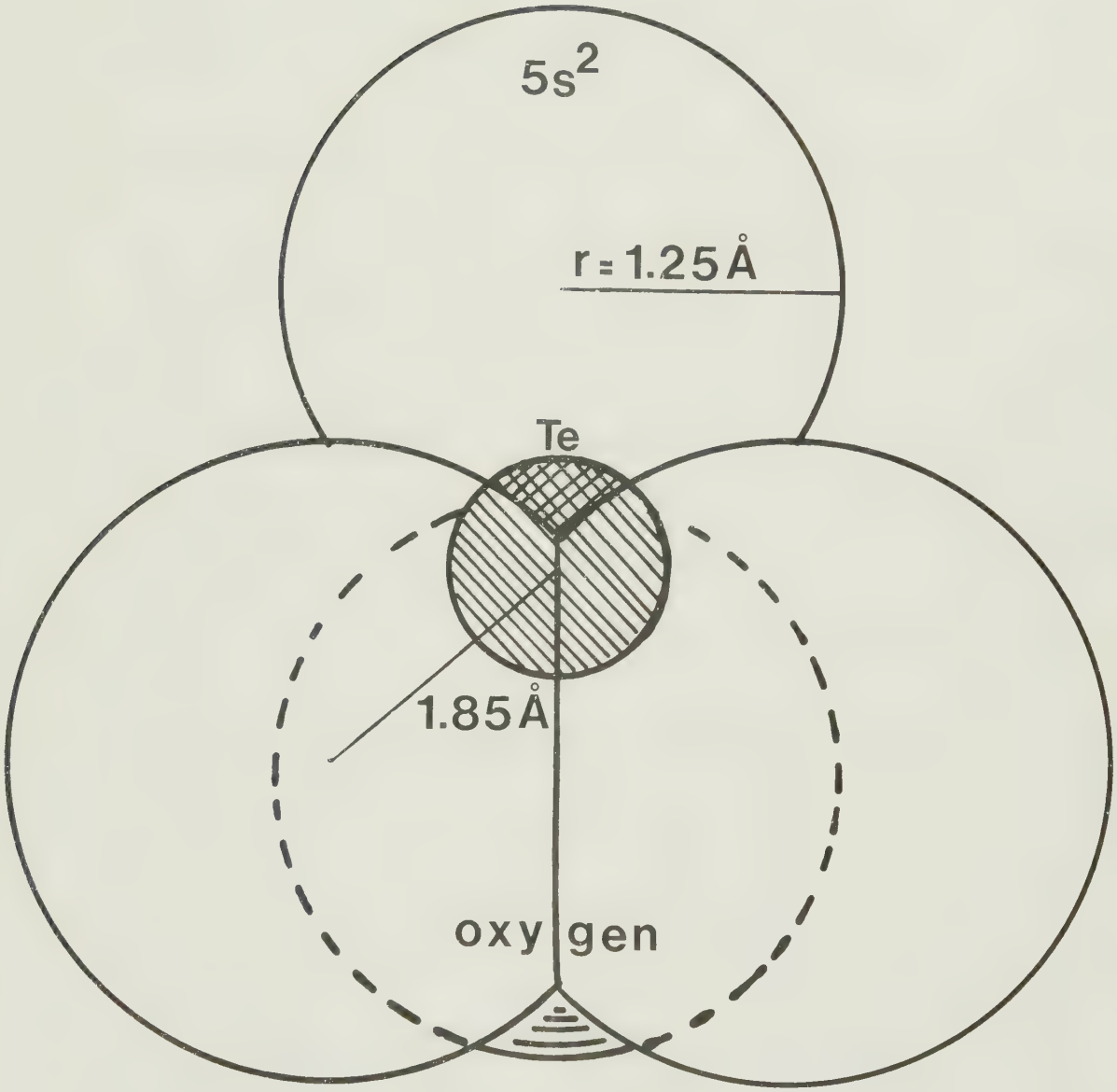

Fig. 18. A model of the TeO_3^{2-} ion with its free electron pair, as obtained from $K_2TeO_3 \cdot 3H_2O$. The action volume of the non-bonding $5s^2$ pair is probably not spherical and the figure only indicates the relative dimensions.

As mentioned above, the mean Te - O distance in $K_2TeO_3 \cdot 3H_2O$ is 1.851(3) Å. If the reported value for O^{2-}, 1.40 Å (Shannon and Prewitt, 1969) is added to the ionic radius of Te(IV), 0.46 Å (Galy, Meunier, Åström and Andersson, 1975) (cf. also Fig. 20) 1.86 Å is obtained which agrees well with 1.851 Å.

b) Comparison between the SO_3^{2-}, SeO_3^{2-} and TeO_3^{2-} ions

It is also of interest to compare the interatomic bond distances and bond angles in the three ions SO_3^{2-}, SeO_3^{2-} and TeO_3^{2-}, where the central atoms all have an inert ns^2 electron pair, n = 3, 4 and 5, respectively. Larsson, Kierkegaard and Nyberg (1972) describe the structure of Na_2SO_3 as being of ionic character, the pyramidal sulphite ion having three-fold symmetry with S - O of 1.504(3) Å and O - S - O of 105.7(2)° (Larsson and Kierkegaard, 1969).

$MgSeO_3 \cdot 6H_2O$ (Weiss, Wendling and Grandjean, 1966) consists of pyramidal SeO_3^{2-} ions and octahedral $[Mg(H_2O)_6]^{2+}$ ions. The oxygen coordination around the Se(IV)-atom is described by the three-fold axis on which the Se-atom is situated. The Se - O bond distance is 1.69(1) Å and the O - Se - O angle is 100.7(5)°. These values for the SeO_3^{2-} ion have been confirmed by Kohn, Inoue, Horie and Akimoto (1976), who have synthesized $MeSeO_3$ (Me = Mg, Mn, Co, Ni, Cu, Zn) hydrothermally and solved the crystal structures. These authors obtained mean values of the Se - O distance and O - Se - O angle of 1.719 Å and 104.3°, respectively.

The SO_3^{2-} and SeO_3^{2-} ions may be compared with the TeO_3^{2-} ion in $K_2TeO_3 \cdot 3H_2O$, where the average Te - O distance and O - Te - O angle

are 1.851(3) Å and 99.3(1)°, respectively. Obviously when going down in the oxygen group in the Periodic Table the A - O bond distance tends to increase while the O - A - O angle in the AO_3^{2-} ion tends to decrease (where A = S, Se and Te). This phenomenon can be explained by the increase in size of S(IV), Se(IV) and Te(IV) ions from S(IV) to Te(IV). The SO_3^{2-} ion is therefore the most flattened trigonal pyramid (cf. Table 5).

c) Three-fold coordination in condensed tellurates(IV)

In most of the tellurate(IV) structures found in the literature tellurium has neither pure three-fold nor pure four-fold coordination. Instead an intermediate between these two types of coordination often occurs, with the fourth Te(IV) - O distance from 2.2 Å to about 2.9 Å. Many tellurate(IV) oxides have two- or three-dimensional network structures and it is of great importance for their construction and stability that the longer tellurium(IV) oxygen bond distances can vary (Lindqvist, 1973). Some recent investigations are listed in Table 6, showing coordination bond distances and angles for different tellurate(IV) structures.

Zemann (1971) found that there also exist one to three weaker interactions with oxygen in a direction which is almost constant with respect to the three strongest bonds. These observations have later been confirmed by Lindqvist (1973), and $Al_2(OH)_2TeO_3SO_4$, $Te_2O_3SO_4$ and $Cu(NH_3)TeO_3 \cdot H_2O$ (Papers I, II and III) all exhibit such longer bonds in a position opposite the three pyramidally coordinated oxygen atoms. The longer "back-bonding" oxygen atoms are situated in the range 2.26 Å - 3.24 Å. For $Te_2O_3SO_4$ there is even a seventh oxygen atom

Table 5. Distances (Å) and angles (°) for S-O, Se-O and Te-O in Na_2SO_3, $MgSeO_3 \cdot 6H_2O$ and $K_2TeO_3 \cdot 3H_2O$.

	Na_2SO_3 [a]	$MgSeO_3 \cdot 6H_2O$ [b]	$K_2TeO_3 \cdot 3H_2O$ [c]
Me - O_1	1.504(3)	1.69(1)	1.848(8)
Me - O_2	1.504(3)	1.69(1)	1.852(6)
Me - O_3	1.504(3)	1.69(1)	1.852(6)
mean value [d]:	1.504(3)	1.69(1)	1.851(3)
O_1 - Me - O_2	105.69(17)	100.7(5)	97.7(3)
O_1 - Me - O_3	105.69(17)	100.7(5)	97.7(3)
O_2 - Me - O_3	105.69(17)	100.7(5)	102.4(4)
mean value [d]:	105.69(17)	100.7(5)	99.3(1)

Me = Na, Mg, K

a) Larsson and Kierkegaard, 1969.

b) Weiss, Wendling and Grandjean, 1966.

c) Paper IV.

d) Hamilton, 1972.

at 3.07 Å. Another interesting fact is that, three of the four strongest coordinated O atoms lie within the same plane, while the fourth oxygen atom is perpendicular to this plane. The most probable explanation for this special configuration is the packing of the structure. As described earlier $Te_2O_3SO_4$ consists of layers connected by van der Waals forces. These layers are built up from Te_2O_5 groups sharing two oxygen atoms with one sulphate tetrahedron. In order to accomodate these sulphate ions the layers have to twist, the unusual configuration thus being due to the strongly coordinated SO_4 units.

d) Four-fold coordination in condensed tellurates(IV)

In four-fold coordinated tellurate(IV) compounds the coordination polyhedron may be described as a trigonal bipyramid with two oxygen atoms in the axial positions and the other two O atoms at two of the three equatorial corners (cf. Fig. 19). The third corner is occupied by the free $5s^2$ electron pair. In $Te(C_6H_4O_2)_2$ (Lindqvist, 1967) it is possible to find isolated TeO_4 units with Te - O bond distances in the range 1.977(22) Å - 2.110(23) Å. However, these isolated TeO_4 units are surrounded by carbon rings of the catecholate groups and are probably influenced by geometrical strains from them. Another structure where the distorted bipyramidal configuration is quite clear is that of α - TeO_2 (Lindqvist, 1968), where the equatorial oxygen - tellurium(IV) bond distances are significally shorter (1.90(2) Å) than the axial ones (2.08(2) Å). In comparison with $(NH_4)_2Te_2O_5 \cdot 2H_2O$ (Paper V), where it is possible to consider the two independent tellurium(IV) atoms as having four-fold coordination, the difference is that the two longest axial Te - O bond distances

Table 6. Distances and angles in 71 different tellurium(IV)-oxygen coordination polyhedra. The four closest oxygen atoms are considered. The latest corresponding compilation comprise 30 polyhedra (Lindqvist, 1973).

Compound	Ref.	Te–O bond distances			
		$Te–O_a$	$Te–O_b$	$Te–O_c$	$Te–O_d$
$Co_6Te_5O_{16}(Te_4)$	65	1.888(9)	1.921(9)	2.060(9)	2.06(9)
α–TeO_2	41	1.90(2)	1.90(2)	2.08(2)	2.08(2)
Te_2O_5	46	1.892(6)	1.913(4)	2.072(5)	2.080(6)
$Te_2O_3(HPO_4)(Te_2)$	49	1.83(4)	1.87(4)	2.04(4)	2.09(4)
$MoTe_2O_7(Te_1)$	1	1.886(5)	1.898(5)	2.079(5)	2.099(5)
$Te_3Nb_2O_{11}(Te_2)$	18	1.84(2)	1.84(2)	2.10(2)	2.10(2)
$Zn_2Te_3O_8(Te_1)$	24	1.83(3)	1.83(3)	2.10(3)	2.10(3)
$H_2Te_2O_6$	47	1.861(6)	1.937(4)	2.065(5)	2.107(5)
$CaTe_3O_8$	69	1.910	1.956	2.102	2.110
$Te(C_6H_4O_2)_2$	40	1.98(2)	1.98(2)	2.01(3)	2.11(2)
$Te_2O_3(HPO_4)(Te_1)$	49	1.79(4)	1.99(4)	2.02(4)	2.12(4)
$TiTe_3O_8$	53	1.85(2)	1.85(2)	2.12(2)	2.12(2)
Te_4O_9	45	1.902(9)	1.883(8)	2.020(9)	2.144(8)
$NaVTeO_5$	11	1.93(5)	1.94(3)	2.04(3)	2.15(3)
$Te_2O_4 \cdot HNO_3$	63	1.88(2)	1.95(1)	2.02(2)	2.16(2)
$UO_2Te_3O_7$	19	1.78(4)	2.02(4)	2.15(4)	2.16(4)
β–TeO_2	4	1.88(2)	1.93(2)	2.07(2)	2.19(2)
$(NH_4)_2Te_2O_5 \cdot 2H_2O(Te_1)$	V	1.834(4)	1.899(3)	2.034(4)	2.218(3)
$MoTe_2O_7(Te_2)$	1	1.862(5)	1.899(5)	2.022(5)	2.233(5)
$UTeO_5$	54	1.88(3)	1.96(3)	1.89(3)	2.24(3)
$Fe_2Te_4O_{11}(Te_4)$	3	1.93	1.98	2.07	2.25

Compound	Ref.	Te-O bond distances			
		$Te-O_a$	$Te-O_b$	$Te-O_c$	$Te-O_d$
$Te_2O_3SO_4$	II	1.89(1)	1.91(5)	2.00(1)	2.26(1)
$Fe_2Te_4O_{11}(Te_1)$	3	1.88	1.93	1.97	2.30
$CaTeO_2(CO_3)$	15	1.85(1)	1.95(1)	2.05(1)	2.31(1)
$CuTeO_3(Te_2)$	42	1.88(2)	1.88(2)	1.96(2)	2.32(2)
$(Mn,Ca,Zn)Te_2O_5$	66	1.84(5)	1.87(2)	2.04(2)	2.36(2)
$Fe(OH)Te_2O_5$	57	1.90(2)	1.90(2)	1.95(4)	2.37(2)
$Fe_2(TeO_3)_2SO_4 \cdot 3H_2O(Te_2)$	58	1.87(2)	1.89(2)	1.91(2)	2.38(2)
$MgTe_2O_5$	64	1.84(1)	1.86(1)	1.97(1)	2.40(1)
$CuTe_2O_5(Te_2)$	26	1.859(3)	1.866(3)	2.019(3)	2.402(3)
$Zn_2Te_3O_8(Te_2)$	24	1.88(3)	1.93(3)	1.98(3)	2.41(3)
$Fe_2Te_4O_{11}(Te_3)$	3	1.80	1.86	2.09	2.43
Mo_5TeO_{16}	2	1.813(6)	1.960(7)	2.019(7)	2.453(7)
$Fe_2Te_4O_{11}(Te_2)$	3	1.78	1.84	2.04	2.49
$\{Fe_2[TeO_3]_3 \cdot H_2O\} \cdot xH_2O(Te_1)$	59	1.81(4)	1.79(4)	1.86(5)	2.50(5)
$(NH_4)_2Te_2O_5 \cdot 2H_2O(Te_2)$	V	1.840(3)	1.870(3)	1.971(4)	2.506(4)
$\{Fe_2[TeO_3]_3 \cdot H_2O\} \cdot xH_2O(Te_2)$	59	1.87(4)	1.84(4)	1.87(4)	2.52(4)
$H_3Fe_2(TeO_3)_4Cl(Te_2)$	13	1.88(7)	1.91(5)	1.87(6)	2.54(6)
$Cr_2Te_4O_{11}(Te_2)$	52	1.846(9)	1.89(1)	1.89(1)	2.56(1)
$Al_2(OH)_2TeO_3SO_4$	I	1.902(4)	1.939(3)	1.902(3)	2.567(3)
$Fe(OH)TeO_3 \cdot H_2O(Te_2)$	12	1.86(1)	1.91(1)	1.89(1)	2.57(1)
α-$TeVO_4$	51	1.81(3)	1.95(3)	1.99(3)	2.58(3)
$Fe_2Te_3O_9(Te_3)$	3	1.84	1.84	1.87	2.59
$Co_6Te_5O_{16}(Te_3)$	65	1.858(9)	1.858(9)	1.894(9)	2.593(9)
$CuTe_2O_5(Te_1)$	26	1.877(3)	1.931(3)	1.883(3)	2.607(3)
$Co_6Te_5O_{16}(Te_1)$	65	1.866(9)	1.866(9)	1.863(9)	2.615(9)

Compound	Ref.	Te-O bond distances			
		$Te-O_a$	$Te-O_b$	$Te-O_c$	$Te-O_d$
Fe_2TeO_5	3	1.890(9)	1.868(8)	1.950(9)	2.632(9)
$Te_2V_2O_9$	51	1.843(3)	1.862(3)	1.921(3)	2.681(3)
$Fe(TeO_3)_2SO_4 \cdot 3H_2O(Te_1)$	58	1.85(2)	1.91(2)	1.99(2)	2.70(2)
$CoTeO_3$	35	1.902	1.920	1.920	2.704
$CuTeO_3(Te_1)$	42	1.89(2)	1.89(2)	1.86(2)	2.71(2)
$ZnTeO_3$	25	1.88(3)	1.90(3)	1.86(3)	2.71(3)
$Cr_2Te_4O_{11}(Te_1)$	52	1.856(9)	1.872(9)	1.881(8)	2.719(7)
$Fe(OH)TeO_3 \cdot H_2O(Te_1)$	12	1.89(1)	1.89(1)	1.89(1)	2.74(1)
$\{Fe_2[TeO_3]_3 \cdot H_2O\} \cdot xH_2O(Te_3)$	59	1.85(5)	1.81(3)	1.97(4)	2.75(4)
$BaTeO_3$	17	1.856	1.856	1.879	2.785
$Co_6Te_5O_{16}(Te_2)$	65	1.904(9)	1.833(9)	1.904(9)	2.805(9)
$Fe_2Te_3O_9(Te_1)$	3	1.85	1.85	1.90	2.84
$Co_3Te_2O_6(OH)_2(Te_1)$	56	1.89(1)	1.90(1)	1.90(1)	2.84(6)
$Fe_2Te_3O_9(Te_2)$	3	1.85	1.90	1.90	2.90
$Ni_3Te_2O_6(OH)(Te_2)$	56	1.73(4)	1.73(4)	1.73(4)	2.90(4)
$[(Zn,Fe)_2(TeO_3)_3]Na_xH_{2-x} \cdot yH_2O$	50	1.90(2)	1.92(3)	1.90(2)	2.91(3)
$H_3Fe_2(TeO_3)_4Cl(Te_1)$	13	1.86(5)	1.91(7)	1.91(3)	2.93(6)
$Co_3Te_2O_6(OH)_2(Te_2)$	56	1.91(1)	1.91(1)	1.91(1)	2.94(1)
$Ni_3Te_2O_6(OH)_2(Te_1)$	56	1.86(5)	1.86(5)	1.99(3)	2.94(7)
$Cu(NH_3)TeO_3 \cdot H_2O$	III	1.877(7)	1.870(7)	1.885(8)	2.950(7)
$CuTeO_3 \cdot 2H_2O$	14	1.86(1)	1.86(1)	1.89(1)	2.98(1)
$Te_3Nb_2O_{11}(Te_1)$	18	1.86(2)	1.86(2)	1.84(2)	3.03(2)
$BaTeO_3 \cdot H_2O$	60	1.858(6)	1.859(6)	1.847(7)	3.035(7)
Li_2TeO_3	16	1.85(2)	1.87(2)	1.93(2)	3.19(2)
$K_2TeO_3 \cdot 3H_2O$	IV	1.848(8)	1.852(6)	1.852(6)	3.872(8)

Table 6. Continued.

Compound	Ref.	O-Te-O angles (°)						Mean σ
		a,b	a,c	a,d	b,c	b,d	c,d	
$Co_6Te_5O_{16}(Te_4)$	65	113	81	81	83	83	151	0.3
α-TeO_2	41	102	85	88	88	85	169	1.2
Te_2O_5	46	91	86	87	89	82	166	0.2
$Te_2O_3(HPO_4)(Te_2)$	49	95	82	85	88	95	168	2.0
$MoTe_2O_7(Te_1)$	1	101	88	87	99	77	151	0.5
$Te_3Nb_2O_{11}(Te_2)$	18	88	90	92	92	90	177	0.9
$Zn_2Te_3O_8(Te_1)$	24	106	84	93	93	84	175	1.5
$H_2Te_2O_6$	47	91	90	87	86	84	172	0.2
$Te(C_6H_4O_2)_2$	40	98	85	81	81	80	154	1.0
$Te_2O_3(HPO_4)(Te_1)$	49	91	81	88	83	89	166	2.0
$TiTe_3O_8$	53	102	80	86	86	80	159	1.5
Te_4O_9	45	99	88	90	91	82	172	0.3
$NaVTeO_5$	11	94	91	79	88	86	167	1.4
$Te_2O_4 \cdot HNO_3$	63	100	82	85	81	73	148	0.8
$UO_2Te_3O_7$	19	96	89	83	68	91	157	2.0
$(NH_4)_2Te_2O_5 \cdot 2H_2O(Te_1)$	V	102	90	88	88	76	163	0.1
β-TeO_2	4	101	90	78	90	90	168	1.0
$MoTe_2O_7(Te_2)$	1	101	99	84	99	81	159	0.5
$UTeO_5$	54	102	81	83	74	85	151	1.0
$Fe_2Te_4O_{11}(Te_4)$	3	99	81	70	93	86	150	3.0
$Te_2O_3SO_4$	II	112	86	143	78	86	131	0.4
$Fe_2Te_4O_{11}(Te_1)$	3	97	108	86	81	74	155	3.0
$CaTeO_2(CO_3)$	15	98	91	78	78	145	68	0.5

Compound	Ref.	O-Te-O angles (°)						Mean σ
		a,b	a,c	a,d	b,c	b,d	c,d	
$CuTeO_3(Te_2)$	42	106	86	92	86	92	176	0.8
$(Mn,Ca,Zn)Te_2O_5$	66	98	90	88	85	76	160	2.0
$Fe(OH)Te_2O_5$	57	96	92	71	92	87	162	1.0
$Fe_2(TeO_3)_2SO_4 \cdot 3H_2O(Te_2)$	58	88	105	82	104	68	170	1.0
$MnTe_2O_5$	64	98	94	77	96	99	163	0.5
$CuTe_2O_5(Te_2)$	26	99	87	80	89	93	167	0.1
$Zn_2Te_3O_8(Te_2)$	24	98	94	83	80	77	156	1.5
$Fe_2Te_4O_{11}(Te_3)$	3	96	96	86	101	86	176	3.0
Mo_5TeO_{16}	2	98	95	96	77	67	143	0.3
$Fe_2Te_4O_{11}(Te_2)$	3	95	92	83	96	55	170	3.0
$\{Fe_2(TeO_3)_3 \cdot H_2O\} \cdot xH_2O(Te_1)$	59	98	94	81	90	71	160	1.9
$(NH_4)_2Te_2O_5 \cdot 2H_2O(Te_2)$	V	102	95	86	89	77	165	0.1
$\{Fe_2(TeO_3)_3 \cdot H_2O\} \cdot xH_2O(Te_2)$	59	96	92	84	91	74	164	1.9
$H_3Fe_2(TeO_3)_4Cl(Te_2)$	13	97	88	76	99	89	102	3.0
$Cr_2Te_4O_{11}(Te_1)$	52	96	93	78	97	89	169	0.4
$Cr_2Te_4O_{11}(Te_2)$	52	96	93	71	96	94	162	0.5
$Al_2(OH)_2TeO_3SO_4$	I	94	94	67	91	121	150	0.1
$Fe(OH)TeO_3 \cdot H_2O(Te_2)$	12	96	94	81	92	70	161	0.5
α-$TeVO_4$	51	92	99	101	94	84	151	0.8
$Fe_2Te_3O_9(Te_3)$	3	96	96	86	101	86	176	3.0
$Co_6Te_5O_{16}(Te_3)$	65	100	97	75	97	84	175	0.3
$CuTe_2O_5(Te_1)$	26	93	95	72	91	79	163	0.1
$CoTe_5O_{16}(Te_1)$	65	103	98	76	92	73	162	0.3
Fe_2TeO_5	3	97	91	72	96	64	154	3.0
$Te_2V_2O_9$	51	100	90	90	95	90	175	0.3

Compound	Ref.	O-Te-O angles (°)						Mean σ
		a,b	a,c	a,d	b,c	b,d	c,d	
$Fe(TeO_3)_2SO_4 \cdot 3H_2O(Te_1)$	58	97	91	89	88	72	160	1.0
$CoTeO_3$	35	103	103	78	92	72	164	3.0
$CuTeO_3(Te_1)$	42	93	96	70	96	70	158	0.8
$ZnTeO_3$	25	98	95	89	95	71	166	1.5
$Fe(OH)TeO_3 \cdot H_2O(Te_1)$	12	94	96	96	100	87	167	0.5
$\{Fe_2(TeO_3)_3 \cdot H_2O\} \cdot xH_2O(Te_3)$	59	96	100	71	93	69	154	1.7
$BaTeO_3$	17	98	100	89	100	89	167	0.5
$Co_6Te_5O_{16}(Te_2)$	65	93	93	72	96	70	158	0.3
$Fe_2Te_3O_9(Te_1)$	3	98	96	75	96	70	162	3.0
$Fe_2Te_3O_9(Te_2)$	3	98	98	70	90	77	160	3.0
$Co_3Te_2O_6(OH)_2(Te_1)$	56	98	98	75	98	68	163	0.5
$Ni_3Te_2O_6(OH)_2(Te_2)$	56	96	96	73	96	73	162	3.0
$[Zn,Fe)_2(TeO_3)_3]Na_xH_{2-x} \cdot yH_2O$	50	97	94	73	97	69	160	0.9
$H_3Fe_2(TeO_3)_4Cl(Te_1)$	13	102	97	68	90	65	146	3.0
$CuTeO_3 \cdot 2H_2O$	56	102	98	59	96	106	150	3.0
$Co_3Te_2O_6(OH)_2(Te_2)$	56	95	95	75	95	75	166	0.7
$Ni_3Te_2O_6(OH)_2(Te_1)$	III	109	98	65	98	65	164	2.0
$Te_3Nb_2O_{11}(Te_1)$	14	91	97	106	91	81	156	0.7
$Cu(NH_3)TeO_3 \cdot H_2O$	18	98	96	69	95	116	147	0.3
$BaTeO_3 \cdot H_2O$	60	96	99	73	103	87	169	0.3
Li_2TeO_3	16	101	99	71	100	71	164*	0.9
$K_2TeO_3 \cdot 3H_2O$	IV	102	98	74	98	74	165	0.3

*recalculated

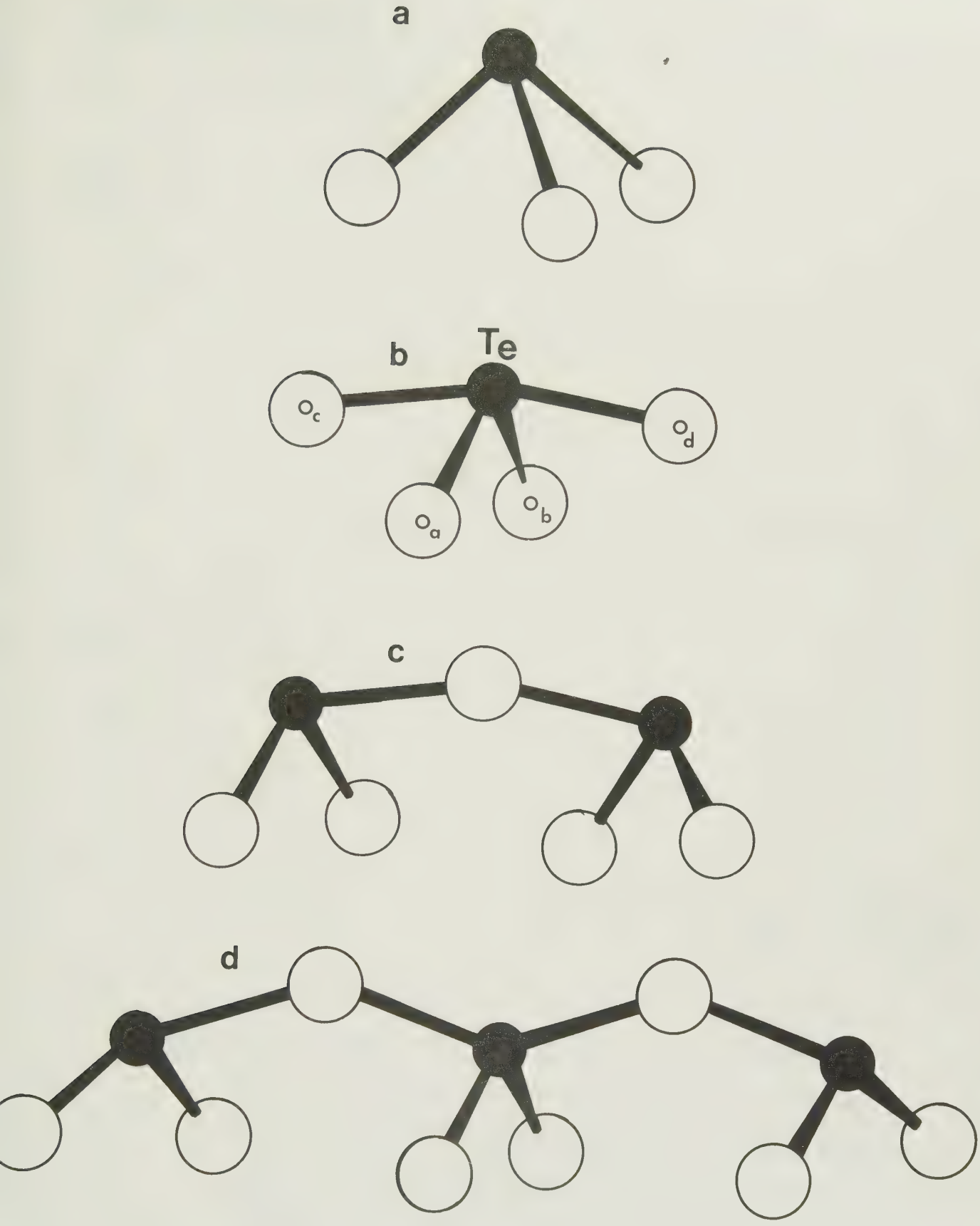

Fig. 19. Coordination of tellurium(IV). a) and b) illustrate three- and four-fold coordination, respectively. c) and d) show Te_2O_5- and Te_3O_8-units.

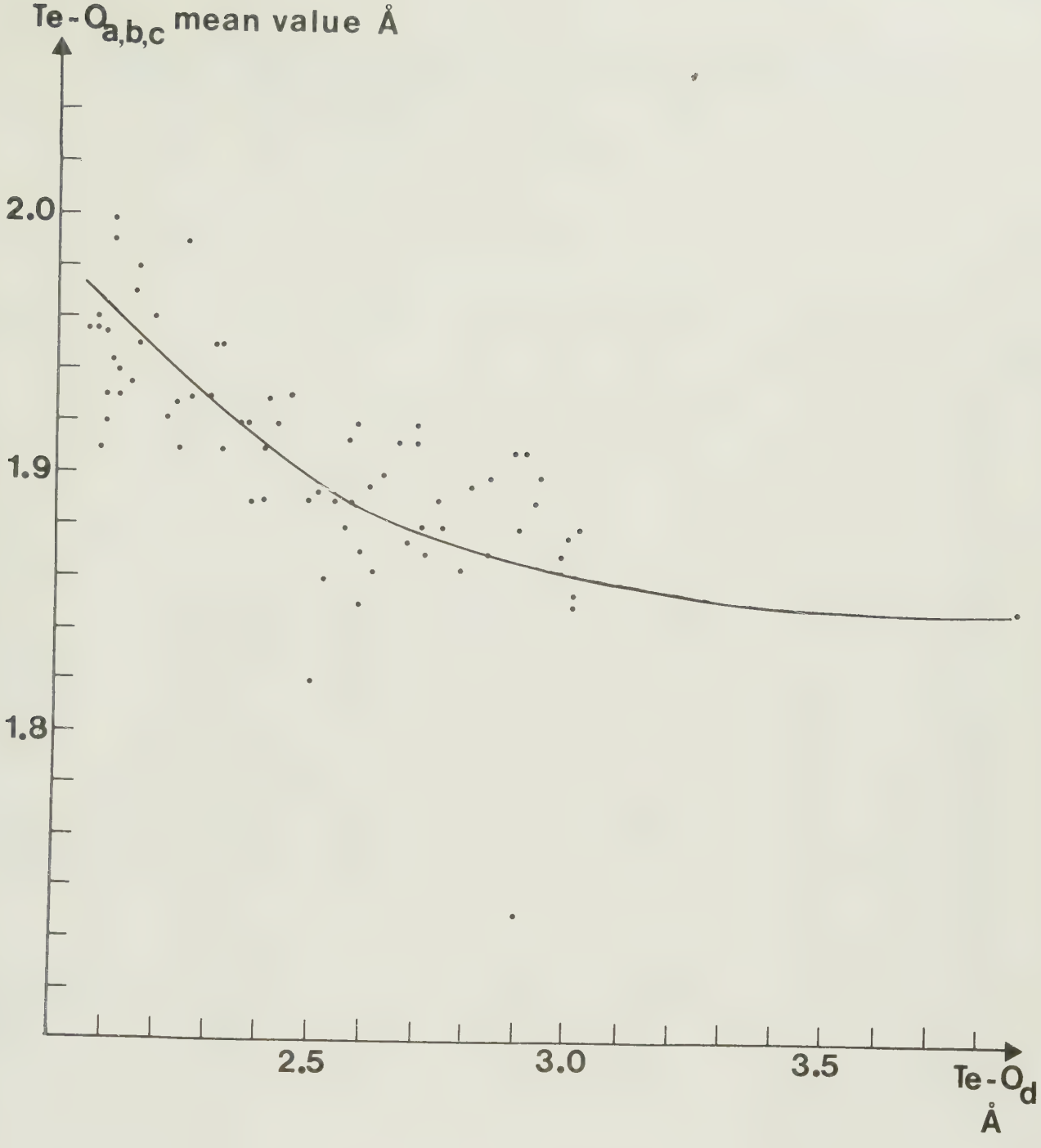

Fig. 20. A curve showing the Te - O_d distance as a function of the mean value of the three Te - $O_{a,b,c}$ distances in the tellurium(IV) - oxygen polyhedra (cf. Table 6 and Fig. 19). The diagram shows the tendency of the Te - O distance in the unpolarized TeO_3^{2-} ion as contained in $K_2TeO_3 \cdot 3H_2O$ (Paper IV).

Table 7. Four-fold oxygen coordination of tellurates(IV). The compounds are listed in order of the longest Te - O_{ax} bond.

ompound	Te - O_{eq} Å	Te - O_{ax} Å	O_{eq}-Te-O_{eq} °	O_{ax}-Te-O_{ax} °	Re
e_2O_5	1.892(6), 1.913(4)	2.072(5), 2.080(6)	91	166	43
-TeO_2	2 x 1.90(2)	2 x 2.10(2) Å	102	169	38
$n_2Te_3O_8$	2 x 1.83(3)	2 x 2.10(3)	106	175	22
$e_3Nb_2O_{11}$	2 x 1.84(2)	2 x 2.10(2)	86	183	17
$_2Te_2O_6$	1.861(6), 1.937(4)	2.065(5), 2.107(5)	91	172	44
$e(C_6H_4O_2)_2$	1.98(2), 1.98(2)	2.01(3), 2.11(3)	98	154	37
$e_2O_3(HPO_4)$	1.79(4), 1.99(4)	2.02(4), 2.12(4)	95	168	46
iTe_3O_8	2 x 1.85(2)	2 x 2.12(2)	102	159	50
$e_2O_4 \cdot HNO_3$	1.88(2), 1.95(1)	2.02(2), 2.16(2)	100	148	60
$O_2Te_3O_7$	1.78(4), 2.02(4)	2.15(4), 2.16(4)	96	157	18
-TeO_2	1.88(2), 1.93(2)	2.07(2), 2.19(2)	101	168	
$NH_4)_2Te_2O_5 \cdot 2H_2O$	1.834(4), 1.899(3)	2.034(3), 2.218(3)	102	163	
$'e_2O_3SO_4$	1.89(1), 1.914(5)	2.00(1), 2.26(1)	112	131	II
$JTeO_5$	1.88(3), 1.96(3)	1.89(3), 2.24(3)	102	151	5

Table 8. Tellurates(IV) containing Te_2O_5 groups.

Compound	Angle (°) Te(1)-O-Te(2)	Distances (Å) Te(1)-O	Te(2)-O	Ref.
$(Mn,Ca,Zn)Te_2O_5$	128.3	2.04	2.36	63
$Fe(OH)Te_2O_5$	118.4	1.95	1.95	54
$Fe_2Te_4O_{11}$	132	1.98	2.10	3
$CuTe_2O_5$	120.6	1.931(3)	2.019(3)	23
$Zn_2Te_3O_8$	126.0 (2x)	1.98	2.10	22
$Te_2V_2O_9$	143.3	1.921(3)	1.921(3)	48
$(NH_4)_2Te_2O_5 \cdot 2H_2O$	118.0	2.030(3)	1.901(3)	V
$Nb_2Te_3O_{11}$	132.1 (2x)	1.84	2.10	17
$MgTe_2O_5$	121	1.97	1.97	61
$Te_2O_3SO_4$	134.9	1.914	1.914	II
$Cr_2Te_4O_{11}$	179.9	1.885	1.885	49

are longer than in α - TeO_2 or in $Te_2O_4 \cdot HNO_3$ (Swink and Carpenter, 1966), which also contains four-coordinated Te(IV) atoms. A comparison between axial and equatorial Te - O distances in four-coordinated tellurates(IV) is given in Table 7.

e) Te_2O_5 and Te_3O_8 units in condensed tellurates(IV)

The first tellurium(IV) structure found to contain Te_2O_5 units is Denningite, $(Mn,Ca,Zn)Te_2O_5$ (Walitzi, 1965). Here it was possible to study isolated Te_2O_5 groups (cf. Fig. 19) connected to form chains by intermediate Te - O bonds. Since then other tellurate(IV) structures containing Te_2O_5 have been determined and these are compared with $(NH_4)_2Te_2O_5 \cdot 2H_2O$ (Paper V) in Table 8.

Until now only two Te(IV)-compounds containing Te_3O_8 units have been reported in the literature, namely $Zn_2Te_3O_8$ (Hanke, 1966) and $Te_3Nb_2O_{11}$ (Galy and Lindqvist, 1978). These two structures have a similar arrangement of the central Te - O - Te - O - Te chain, both having a two-fold symmetry axis through the central Te atom (cf. Fig. 19).

ACKNOWLEDGEMENTS

I wish to express my sincere gratitude to Professor Oliver Lindqvis for his help and in particular for many stimulating and instructive discussions.

I should also like to thank:
Professor Georg Lundgren for many valuable discussions,
Professor Nils-Gösta Vannerberg for his stimulating interest in this work,
Dr. Jacques Moret for supplying some of the single crystals used in this work and for interesting discussions on hydrothermal syntheses
Dr. Axel Nørlund-Christensen for giving me permission to use his hydrothermal equipment,
Dr. Sten Andersson for help with the construction of the hydrotherm synthesis equipment,
Dr. Lennart Falck for discussions on tellurate problems,
Dr. Susan Jagner for helpful comments and careful revision of the English text,
Mr. Lars Lagerqvist for excellent technical assistance and for drawing the hydrothermal synthesis equipment,
Mrs. Margareta Johansson and Mrs. Gunnel Thorsell for typing the manuscript,
Mr. Algot Alm and Mr. Bo Bergman for offset reproduction of preprin and this thesis.

This work has been supported financially by the Swedish Natural Science Research Council (NFR).

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Reprinted from *Acta Crystallographica*, Vol. B 32, part 2, February 1976

PRINTED IN DENMARK

Acta Cryst. (1976). B32, 407

The Crystal Structure of $Al_2(OH)_2TeO_3SO_4$

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(*Received* 9 *June* 1975; *accepted* 16 *June* 1975)

$Al_2(OH)_2TeO_3SO_4$ crystallizes in space group $P2_1/m$ with $a=7{\cdot}013$ (2), $b=9{\cdot}539$ (4), $c=4{\cdot}880$ (2) Å, $\beta=92{\cdot}65$ (3)°, $Z=2$. The structure was solved from Patterson and electron density calculations with 1289 independent reflexions, and a final R of 0·032 was obtained. The structure consists of tetrahedral SO_4^{2-} ions and pyramidal TeO_3 units connected by Al to form infinite sheets. The Al coordination is approximately octahedral with Al–O distances of 1·864–1·934 Å. The Te–O and the S–O lengths are 1·902–1·939 and 1·467–1·487 Å respectively.

Introduction

A new Te^{IV} compound, $Al_2(OH)_2TeO_3SO_4$, has been prepared as part of an investigation of tellurate(IV,VI) chemistry under hydrothermal conditions (Moret, 1972) and single crystals were kindly provided by Dr Moret. In most of the previously known M–tellurate(IV) structures, the metal atoms (Zn, Cu, Fe) are involved in three-dimensional covalent M–O–Te^{IV} nets (Lindqvist, 1973; Zeeman, 1971). Only in $BaTeO_3.H_2O$ (Rottersten-Nielsen, Grønbæk-Hazell & Rasmussen, 1971) can the building units be regarded as Ba^{2+} and TeO_3^{2-} ions.

The aim of the present investigation was to examine the effect of the Al atoms on the Te^{IV} coordination.

Data collection

Crystals of $Al_2(OH)_2TeO_3SO_4$ were first investigated with Weissenberg techniques, the reflexion pattern indicating the space groups $P2_1$ or $P2_1/m$. Accurate cell dimensions were determined from a Guinier powder photograph (Table 1) with KCl as an internal standard ($a_{KCl}=6{\cdot}2919_4$ Å at 20°C; Hambling, 1953), (*POWDER*; Lindqvist & Wengelin, 1967). Crystallographic data are given in Table 2. The density was determined by flotation in aqueous thallium(I) formate and malonate ('Clericis Lösung').

The crystal was mounted along **c** (for dimensions see Fig. 1) and intensities were collected on a two-

Table 1. *Powder data for* $Al_2(OH)_2TeO_3SO_4$; Cu $K\alpha_1$ *radiation* (1·54050 Å)

h	k	l	$\sin^2\theta$ (obs)	$\sin^2\theta$ (calc)	d(calc) (Å)	I
1	0	0	0·01213	0·01209	7·006	*vw*
1	1	0	0·01864	0·01861	5·647	*w*
0	2	0	0·02625	0·02608	4·769	*m*
0	1	$\bar{1}$	0·03155	0·03149	4·340	*w*
1	0	$\bar{1}$	0·03566	0·03545	4·091	*w*
1	0	1	0·03859	0·03866	3·917	*m*
1	1	$\bar{1}$	0·04226	0·04197	3·760	*w*
1	1	1	0·04513	0·04518	3·624	*w*
2	1	0	0·05489	0·05487	3·288	*w*
1	2	$\bar{1}$	0·06160	0·06154	3·105	*m*
1	2	1	0·06483	0·06475	3·027	*w*
2	0	$\bar{1}$	0·07020	0·07011	2·909	*m*
1	3	0	0·07087	0·07077	2·895	*w*
2	2	0	0·74061	0·07443	2·823	*w*
2	0	1	0·07646	0·07653	2·784	*s*
2	1	$\bar{1}$	0·07646	0·07663	2·782	*s*
0	3	$\bar{1}$	0·08370	0·08366	2·663	*m*
1	3	$\bar{1}$	0·09424	0·09414	2·510	*m*
0	0	$\bar{2}$	0·10006	0·09988	2·437	*m*
2	2	1	0·10271	0·10261	2·405	*s*
0	4	0	0·10435	0·10433	2·385	*m*
0	1	$\bar{2}$	0·10631	0·10640	2·361	*m*
1	0	$\bar{2}$	0·10887	0·10876	2·269	*w*
1	1	$\bar{2}$	0·11511	0·11528	2·269	*s*
0	4	$\bar{1}$	0·12933	0·12930	2·142	*w*
3	1	$\bar{1}$	0·13514	0·13546	2·093	*vs*
3	0	1	0·13862	0·13858	2·069	*w*
1	4	1	0·14302	0·14299	2·037	*w*
2	0	2	0·15478	0·15466	1·959	*w*
0	3	$\bar{2}$	0·15865	0·15857	1·934	*w*
1	3	2	0·17384	0·17387	1·847	*w*
3	3	1	0·19734	0·19726	1·734	*w*
4	1	0	0·20014	0·19992	1·723	*w*

Table 2. *Crystallographic data for* $Al_2(OH)_2TeO_3SO_4$

$a = 7{\cdot}013$ (2) Å
$b = 9{\cdot}539$ (4)
$c = 4{\cdot}880$ (2)
$\beta = 92{\cdot}65$ (3)°
$V = 326{\cdot}1$ (2) Å^3
$Z = 2$
$M = 359{\cdot}64$
$\varrho_o = 3{\cdot}7$ g cm^{-3}
$\varrho_c = 3{\cdot}66$
Space group: $P2_1/m$
Equivalent positions: $\pm(x, y, z)$; $\pm(x, \frac{1}{2}-y, z)$
μ(Mo $K\alpha$) = 53·4 cm^{-1}
Crystal habit: colourless plates (Fig. 1)

circle single-crystal diffractometer (Pailred) with graphite-monochromated Mo $K\alpha$ radiation. The ω-scanning procedure was used with a scan speed of 2·5° min^{-1}, the background being measured for 24 s at both ends of the scan interval. The layers $hk0$–$hk6$ were recorded up to $2\theta \sim 60°$. 1531 independent reflexions were measured of which 1289 with $\sigma(I)/I < 0{\cdot}4$ were regarded as significant and used in the subsequent analysis. Intensity statistics and Lp corrections were performed with *DATAP*1 (Lindgren, 1975). Absorption effects were calculated with *DATAP*2 (Coppens, Leiserowitz & Rabinovich, 1965). The transmission factors varied from 0·53 to 0·90, but were not applied until a preliminary structure was known.

Structure determination and refinement

The exact chemical composition was not known at the start, but Te and Al were known to be present. From the Patterson function (*DRF*; Zalkin, Berkeley), it was apparent that there were two Te and four Al atoms in the cell occupying positions 2(*e*) and 4(*f*) in space group $P2_1/m$. A complete model was obtained from successive electron density calculations. It then also became obvious that the crystals contained sulphate ions from the $Al_2(SO_4)_3$ solutions used in the preparation.

A refinement based on all 1289 observed reflexions and including anisotropic temperature factors and an isotropic extinction factor (*LINUS*; Coppens & Hamilton, 1970) yielded an R of 0·032. Scattering factors for uncharged Te (Cromer & Waber, 1965), Al, S and O (Doyle & Turner, 1968) corrected for the real part of the anomalous scattering (Cromer, 1965) were used.

Weights $w = (ca/F)^{-1/2}$ for $F \le a$ and $w = [c-(F-a)^{1/2}]^{-1/2}$ for $F \ge a$ gave a reasonable analysis for $a = 30{\cdot}0$ and $c = 50{\cdot}0$ (Table 3).

Table 3. *Weight analysis after the last cycle of refinement*

The quantities $w\Delta^2$ are normalized sums and N is the number of reflexions within each F_o interval.

F_o interval	N	$w\Delta^2$
0·0– 14·2	126	0·90
14·2– 17·8	125	0·73
17·8– 22·0	133	0·71
22·0– 25·4	125	0·68
25·4– 29·0	126	0·55
29·0– 32·7	130	1·10
32·7– 37·8	128	0·84
37·8– 44·7	134	0·91
44·7– 57·1	129	0·93
57·1–136·2	133	2·59

$R = \sum|F_o - |F_c|| / \sum F_o = 0{\cdot}032$
$R_w = (\sum w|F_o - |F_c||^2 / \sum wF_o^2)^{1/2} = 0{\cdot}032$

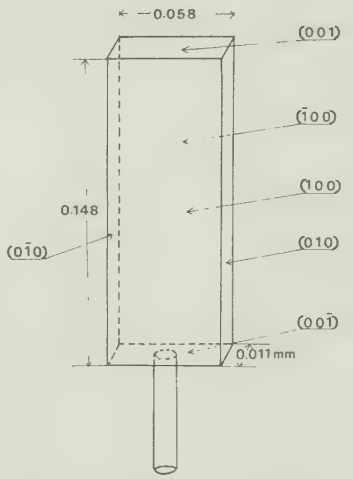

Fig. 1. The crystal used for data collection. The crystal volume is $7{\cdot}56 \times 10^{-4}$ mm^3.

Table 4. *Final atomic parameters in* $Al_2(OH)_2TeO_3SO_4$

The anisotropic temperature factor is $\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2hka^*b^*U_{12} + 2hla^*c^*U_{13} + 2klb^*c^*U_{23})]$.

Estimated standard deviations in parentheses.

	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Te	0·18867 (5)	¼	0·31015 (7)	0·00485 (18)	0·00479 (11)	0·00510 (11)		0·00034 (7)	
Al	0·0544 (2)	0·5752 (1)	0·2552 (2)	0·0080 (2)	0·0044 (5)	0·0066 (5)	0·0004 (5)	0·0007 (3)	0·0000 (3)
S	0·6069 (2)	¼	0·9623 (2)	0·0049 (5)	0·0092 (5)	0·0095 (5)		0·0009 (4)	
O(1)	−0·0067 (6)	¼	0·5801 (8)	0·0139 (16)	0·0080 (16)	0·0037 (16)		0·0031 (11)	
O(2)	0·0686 (4)	0·3920 (3)	0·0887 (5)	0·0109 (11)	0·0030 (10)	0·0062 (11)	0·0008 (8)	−0·0014 (7)	0·0000 (7)
O(3)	0·1682 (4)	0·4846 (3)	0·5657 (5)	0·0045 (10)	0·0091 (11)	0·0085 (11)	−0·0007 (9)	0·0003 (7)	−0·0003 (10)
O(4)	0·4058 (6)	¼	0·8663 (10)	0·0054 (17)	0·0168 (21)	0·0250 (24)		−0·0018 (14)	
O(5)	0·6250 (7)	¼	0·2619 (10)	0·0134 (21)	0·0414 (31)	0·0107 (22)		−0·0008 (15)	
O(6)	0·7031 (4)	0·3760 (3)	0·8528 (7)	0·0106 (12)	0·0095 (12)	0·0221 (16)	−0·0015 (10)	0·0065 (10)	0·0001 (10)

Isotropic extinction parameter (Coppens & Hamilton, 1970): $g \times 10^{-4} = 0{\cdot}031$ (5).

The refinement indicated only small extinction effects, the isotropic extinction parameter g (Coppens & Hamilton, 1970) being $0{\cdot}031\ (5) \times 10^4$. The final parameter list is given in Table 4.*

The structure was checked with a difference synthesis (*FFT*; Ten Eyck, 1973). The maximum residual density of 2·4 e $Å^{-3}$ occurred close to the Te atoms.

Interatomic distances and angles (*DISTAN*; Zalkin, Berkeley) are presented in Table 5.

* A list of structure factors has been deposited with the British Library Lending Division as Supplementray Publication No. SUP 31205 (8 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, White Friars, Chester CH1 1NZ, England.

Table 5. *Coordination distances and angles in* $Al_2(OH)_2TeO_3SO_4$

The notation is in accordance with Figs. 4 and 5.

Te–O(1)		1·939 (4) Å	O(1)–Te–O(2)		94·4 (1)°
Te–O(2)	(2×)	1·902 (3)	O(1)–Te–O(3)	(2×)	67·4 (1)
Te–O(3)	(2×)	2·567 (3)	O(1)–Te–O(4)		169·3 (2)
Te–O(4)		2·705 (5)	O(2)–Te–O′(2)		90·6 (2)
Al–O(1)		1·889 (2)	O(2)–Te–O(3)	(2×)	67·9 (1)
Al–O(2)		1·934 (3)	O(2)–Te–O′(3)	(2×)	149·6 (1)
Al–O′(2)		1·881 (3)	O(2)–Te–O(4)	(2×)	78·1 (1)
Al–O(3)		1·910 (3)	O(3)–Te–O′(3)		121·2 (1)
Al–O′(3)		1·888 (3)	O(3)–Te–O(4)	(2×)	115·8 (1)
Al–O(6)		1·864 (3)	O(1)–Al–O(2)		172·7 (2)
S—O(4)		1·467 (5)	O(1)–Al–O′(2)		98·7 (2)
S—O(5)		1·467 (5)	O(1)–Al–O′(3)		98·0 (2)
S—O(6)	(2×)	1·487 (3)	O(1)–Al–O(3)		84·4 (2)
			O(1)–Al–O(6)		94·7 (2)
			O(2)–Al–O′(2)		78·9 (1)
			O(2)–Al–O′(3)		83·9 (1)
			O(2)–Al–O(3)		89·0 (1)
			O(2)–Al–O(6)		92·3 (1)
			O′(2)–Al–O(3)		96·1 (1)
			O′(2)–Al–O′(3)		162·3 (1)
			O′(2)–Al–O(6)		95·4 (1)
			O(3)–Al–O′(3)		79·9 (1)
			O(3)–Al–O(6)		168·5 (1)
			O′(3)–Al–O(6)		89·1 (1)
			O(4)–S—O(5)		111·0 (3)
			O(4)–S—O(6)	(2×)	109·2 (2)
			O(5)–S—O(6)	(2×)	109·8 (2)
			O(6)–S—O′(6)		107·8 (3)

Discussion

$Al_2(OH)_2TeO_3SO_4$ is not readily classified as either a covalent or an ionic compound. The structure contains TeO_3 pyramids, SO_4 tetrahedra and dimeric Al–O octahedra, $Al_2(OH)_2O_8$. The building units share O atoms to form infinite sheets. (Figs. 2 and 3).

The layers are held together by van der Waals forces.

Table 6. O–O *distances less than* 4 Å

An asterisk indicates interlayer contacts, and the notation *–A–* means that both O atoms belong to the coordination polyhedron of *A*.

O(6)–O(6)	2·403 (6) Å	–S–
O(4)–O(6) (2×)	2·407 (5)	–S–
O(5)–O(6) (2×)	2·416 (5)	–S–
O(4)–O(5)	2·419 (7)	–S–
O(2)–O(2)	2·424 (5)	–Al–
O(3)–O(3)	2·434 (5)	–Al–
O(1)–O(3) (2×)	2·553 (3)	–Al–
O(2)–O(3)	2·555 (4)	–Al–
O(3)–O(6)	2·663 (4)	–Al–
O(2)–O(3)	2·695 (4)	–Al–
O(2)–O(2)	2·705 (5)	–Te–
O(2)–O(6)	2·740 (4)	–Al–
O(1)–O(6) (2×)	2·761 (5)	–Al–
O(2)–O(6)	2·769 (4)	–Al–
O(2)–O(3)	2·819 (4)	–Al–
O(1)–O(2) (2×)	2·819 (4)	–Te–
O(1)–O(3) (2×)	2·851 (3)	–Al–
O(1)–O(2) (2×)	2·860 (4)	–Al–
O(1)–O(5)	2·948(6)	
O(2)–O(4) (2×)	2·970 (5)	*
O(3)–O(5) (2×)	3·020 (4)	
O(3)–O(4) (2×)	3·114 (4)	*
O(5)–O(6) (2×)	3·146 (6)	
O(1)–O(4)	3·155 (6)	*
O(3)–O(6)	3·227 (4)	
O(4)–O(5)	3·379 (7)	
O(2)–O(5) (2×)	3·533 (5)	
O(2)–O(3)	3·725 (4)	–Al–
O(3)–O(6)	3·755 (4)	–Al–
O(2)–O(6)	3·764 (4)	
O(1)–O(2) (2×)	3·816 (3)	–Al–
O(4)–O(6) (2×)	3·911 (4)	*

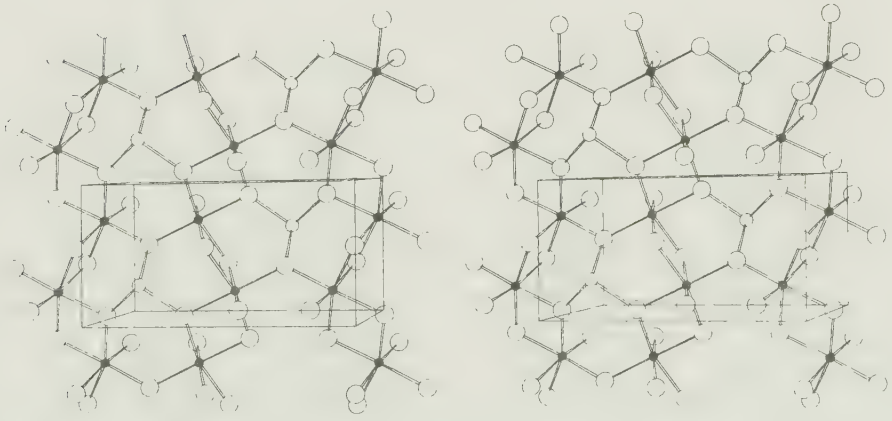

Fig. 2. A stereoscopic view along **a** showing how the dimeric Al–O octahedra are connected by the TeO_3 groups to form infinite sheets (*ORTEP*; Johnson, 1965).

The positions of the sulphate groups give the sheets a bulky shape (Fig. 3) which may stabilize the ordered packing. The sulphate O(4) is involved in short interlayer O–O van der Waals contacts (Table 6). It is also possible that weak Te^{IV}–O interactions contribute slightly to the bonding. The Te^{IV}–O(4) distance is only 2·705 (5) Å, which is comparable to the 2·64 (2) found for similar interactions in $Te(C_6H_4O_2)_2$ (Lindqvist, 1967) and 2·706 (4) Å in Te_2O_5 (Lindqvist & Moret, 1973). In these two compounds there was reason to consider such Te^{IV}–O distances as weak bonds.

The H atom positions could not be deduced from the X-ray investigation, but it is reasonable to assume that they are attached to O(3) atoms, which form bridges between two Al atoms (Fig. 4). Similar double Al$\langle^{OH}_{OH}\rangle$Al bridges have been found in diaspore (Busing & Levy, 1958) and in $[Al_2(OH)_2(H_2O)_8](SO_4)_2.2H_2O$ and the corresponding selenate (Johansson, 1962); the bridging hydroxide groups participated only in weak hydrogen bonds. In $Al_2(OH)_2TeO_3SO_4$ only one of the distances O(3)–O(5) (intralayer) of 3·020 or O(3)–O(4) (interlayer) of 3·114 may correspond to a hydrogen bond (Table 6). However, since both distances are long, it is doubtful if there are any hydrogen bonds in the structure.

The octahedral Al coordination includes, apart from the two O(3) bridge bonds, O atoms from three different TeO_3 groups and one sulphate O (Figs. 2 and 4, Table 5). The Al–O distances are similar to the 1·851 (2)–1·980 (3) in diaspore (Busing & Levy, 1958) and the 1·85–1·95 Å (Johansson, 1962) in $[Al_2(OH)_2(H_2O)_8](SO_4)_2.2H_2O$ (Fig. 4). The dimeric anion $[Al_2(OH)_2(H_2O)_8]^{4-}$ has a very short O–O distance across the double bridge of 2·39 Å. The corresponding value for $Al_2(OH)_2TeO_3SO_4$ is only slightly longer, 2·434 (5) Å.

The coordination of Te is threefold pyramidal (Fig. 5, Table 5), similar to that found in other tellurates(IV) (Zeeman, 1971; Lindqvist, 1973) with Te–O distances of 1·85–2·00 Å. In addition, there are three longer bonds: Te–O(3) (2×) of 2·567 (3) and Te–O(4) of 2·705 (5) Å.

Generally, the weaker Te^{IV}–O bonds have rather asymmetrical geometry, since the O positions are determined mainly by stronger bonds to other atoms

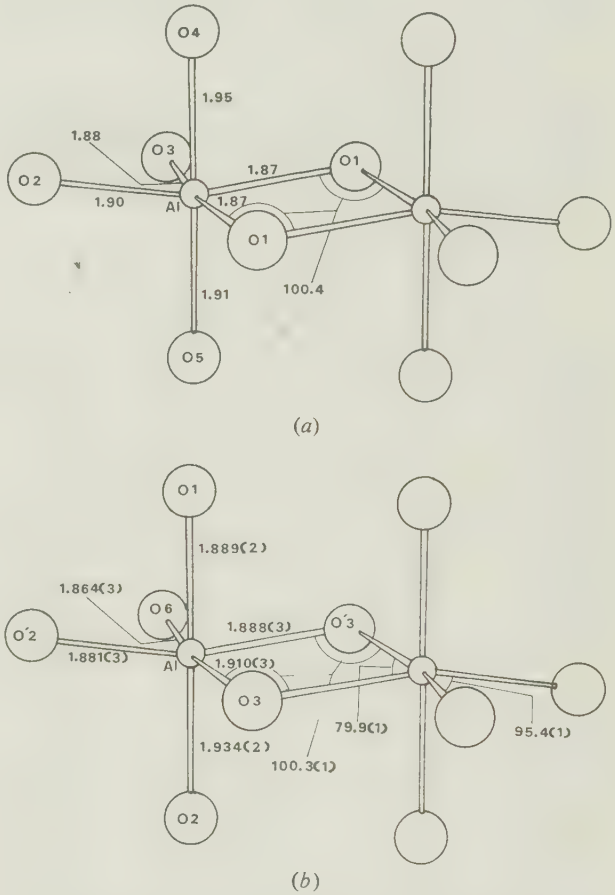

Fig. 4. The O coordination within the dimeric group in (*a*) $[Al_2(OH)_2(H_2O)_8](SO_4)_2.2H_2O$ and (*b*) $Al_2(OH)_2TeO_3SO_4$. The H atoms are probably bonded to the bridging O atoms.

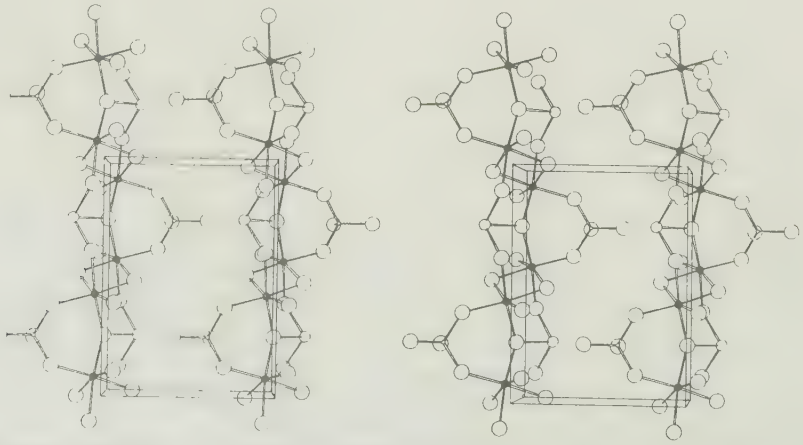

Fig. 3. A stereoscopic drawing of the structure along c showing the adjacent layers of $Al_2(OH)_2TeO_3SO_4$ (*ORTEP*; Johnson, 1965).

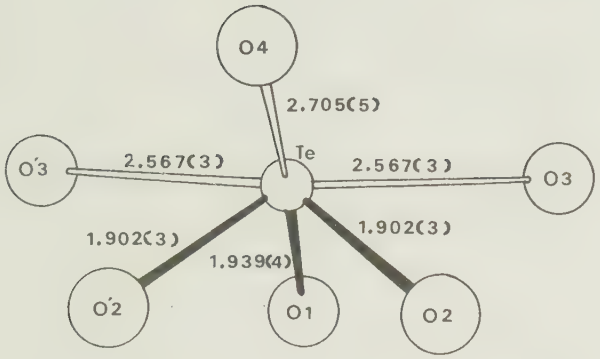

Fig. 5. The O coordination of Te^{IV}.

(Lindqvist, 1973). However, in $Al_2(OH)_2TeO_3SO_4$ the Te^{IV} coordination may be regarded as distorted octahedral. Such octahedral Te^{IV} coordination has been found in $TeCl_4$ (Buss & Krebs, 1971) and $TeCl_3^+AlCl_4^-$ (Krebs, Buss & Altena, 1971) where the short Te–Cl distances are 2·311 and 2·276 Å and the longer ones 2·929 and 3·062 Å, respectively. Buss & Krebs (1971) suggest that this arrangement is due to the ionic character of the structures. Correspondingly, the octahedral distribution of O atoms at short and long distances around Te^{IV} may indicate the presence of TeO_3^{2-} ions in $Al_2(OH)_2TeO_3SO_4$. On the other hand, the Te–O distances in $Al_2(OH)_2TeO_3SO_4$ are slightly longer than those of 1·847 (7)–1·859 (6) Å found in the ionic $BaTeO_3.H_2O$ (Rottersten-Nielsen *et al.*, 1971). This elongation is probably due to the presence of the three weak Te^{IV}–O interactions in $Al_2(OH)_2TeO_3SO_4$, but can also be due to the fact that the TeO_3 oxygen atoms participate in the Al coordination octahedra.

The sulphate groups have the usual bond distances and angles (Table 5). The slight distortion from a regular tetrahedron is presumably due to the fact that O(6) is coordinated to Al.

We thank Professor G. Lundgren for his support and criticism and Dr S. Jagner for revising the English text. Financial aid has been provided by the Swedish Natural Science Research Council (NFR, contract No. 2318).

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Observed and calculated structure factors for $Al_2(OH)_2TeO_3SO_4$. The columns are h, F_o and F_c. Unobserved reflections are indicated with an asterisc.

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2	-	-10*
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-3	-	-2*
-2	18	19
-1	42	43
0	18	18
1	30	-30
2	15	-13
3	17	15
4	31	31

H	11	4
6	18	16
5	21	20
4	-	2*
3	39	-40
2	18	-18
1	-	6*
0	20	19
-1	20	20
-2	30	-29
-3	20	-19
-4	17	19
-5	33	34
-6	33	30

H	10	4
-7	15	-14
-6	22	-23
-5	13	10
-4	44	44
-3	14	11
-2	13	-12
-1	33	-33
0	12	-9
1	34	35
2	15	13
3	15	-12
4	35	-32
5	19	-16
6	25	26

H	9	4
7	-	-4*
6	34	-33
5	40	-41
4	24	-23
3	34	35
2	15	11
1	29	-29
0	42	-42
-1	21	-21
-2	45	47
-3	38	38
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-5	16	-16
-6	29	-29
-7	22	23
-8	32	34

H	8	4
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-7	25	24
-6	35	36
-5	-	-5*
-4	56	-58
-3	18	-17
-2	16	17
-1	27	27
0	15	-14
1	61	-64
2	39	-38
3	-	-4*
4	35	35
5	25	26
6	25	-25
7	21	-20
8	-	7*

H	7	4
8	33	-35
7	-	5*
6	13	13

H	5	4
5	21	20
4	9	9
3	48	-47
2	22	-20
1	25	24
0	43	44
-1	33	32
-2	32	-31
-3	15	-13
-4	15	14
-5	31	29
-6	34	37
-7	25	-25
-8	31	-33
-9	-	0

H	6	4
-9	45	46
-8	-	7
-7	11	-10
-6	29	-29
-5	-	2
-4	41	42
-3	-	-3
-2	31	-31
-1	56	-56
0	24	-24
1	35	35
2	14	13
3	12	-12
4	32	-32
5	13	-12
6	38	37
7	31	29
8	-	4*
9	18	-18

H	5	4
9	-	3*
8	40	41
7	-	7*
6	25	-24
5	29	-29
4	-	2*
3	66	67
2	28	27
1	17	-14
0	42	-43
-1	42	-43
-2	44	44
-3	29	30
-4	22	-22
-5	47	-49
-6	47	-49
-7	15	15
-8	21	22
-9	-	3*

H	4	4
-10	16	-14
-9	33	-41
-8	-	10*
-7	30	31
-6	29	29
-5	27	-27
-4	68	-68
-3	18	-16
-2	17	14
-1	50	52
0	13	13
1	70	-71
2	34	-33
3	24	22
4	51	51
5	28	27
6	30	-30
7	32	-31
8	11	-8
9	25	24

H	3	4
9	-	0*
8	35	-34
7	-	6*
6	45	44
5	59	59
4	35	34
3	34	-33
2	-	3*
1	26	26
0	38	40
-1	29	30
-2	70	-71
-3	58	-58
-4	-	-7*
-5	21	19
-6	22	22
-7	34	-36
-8	28	-28
-9	-	-1*
-10	21	19

H 2 4

-10	13	9
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-8	-	-7*
-7	21	-21
-6	38	-38
-5	-	6*
-4	62	63
-3	23	21
-2	-	-2*
-1	28	-29
0	-	2*
1	65	65
2	31	30
3	-	-8*
4	37	-37
5	22	-21
6	31	29
7	20	19
8	10	-8
9	30	-30

H 1 4

9	-	5*
8	44	44
7	10	7
6	18	-17
5	27	-26
4	-	-5*
3	75	72
2	32	31
1	28	-27
0	61	-61
-1	42	-44
-2	43	44
-3	17	16
-4	22	-18
-5	44	-42
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-7	23	23
-8	34	36
-9	-	1*
-10	17	-17

H 0 4

-10	36	-39
-9	46	-48
-8	-	2*
-7	15	14
-6	36	38
-5	-	-5*
-4	65	-66
-3	-	5*
-2	61	64
-1	74	80
1	57	-57
2	31	-30
3	-	7*
4	50	48
5	27	26
6	48	-47
7	45	-44
8	10	-9
9	22	22
10	22	22

H 13 5

2	9	8
1	27	26
0	16	16
-1	25	-25
-2	26	-26
-3	-	-2*

H 12 5

-5	13	-11
-4	18	15
-3	39	40
-2	12	11
-1	10	-10
0	25	-24
1	-	-9*
2	31	31
3	14	13
4	17	-16

H 11 5

5	10	7
4	33	34
3	12	10
2	19	-18
1	37	-38
0	25	-26
-1	20	19
-2	-	10*
-3	38	-37
-4	38	-37
-5	22	-23
-6	23	20

H 10 5

-7	-	1*
-6	26	24
-5	26	26
-4	-	-3*
-3	41	-42
-2	16	-14
-1	12	12
0	25	25
1	-	4*
2	41	-40
3	24	-23
4	-	4*
5	26	25
6	19	18

H 9 5

7	23	22
6	34	33
5	10	10
4	34	-35
3	25	-25
2	8	5
1	24	25
0	-	7*
-1	36	-38
-2	32	-32
-3	11	-8
-4	23	23
-5	28	30
-6	14	-13
-7	20	-20

H 8 5

-8	29	28
-7	11	-9
-6	22	-21
-5	26	-26
-4	-	-4*
-3	39	40
-2	-	5*
-1	29	-29
0	31	-32
1	-	2*
2	47	47
3	23	24
4	-	0*
5	23	-21
6	-	-9*
7	36	35

H 7 5

8	-	2*
7	19	-19
6	30	-29
5	10	-8
4	32	32
3	11	10
2	27	-26
1	42	-42
0	15	-13
-1	38	38
-2	29	28
-3	-	0*
-4	31	-31
-5	28	-29
-6	25	27
-7	31	32
-8	-	2*

H 6 5

-9	20	-19
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-7	14	-12
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-5	14	13
-4	19	-19
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-1	19	17
0	43	43
1	24	23
2	30	-29
3	-	-10*
4	16	16
5	40	38
6	26	25
7	21	-22
8	22	-20

H 5 5

8	13	-13
7	17	15
6	27	26
5	-	1*
4	42	-40
3	19	-17
2	19	19
1	51	52
0	40	40
-1	23	-23
-2	22	-21
-3	15	14
-4	41	41
-5	28	29
-6	22	-21
-7	28	-28
-8	18	-15
-9	13	10

H 4 5

-9	-	7*
-8	34	36
-7	12	-7
-6	34	-36
-5	28	-28
-4	9	9
-3	44	45
-2	-	4*
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1	-	3*
2	64	65
3	32	32
4	15	-10
5	34	-33
6	14	-14
7	32	31
8	20	19
9	-	-2*

H 3 5

9	21	21
8	-	-5*
7	31	-30
6	34	-34
5	-	-1*
4	47	47
3	27	28
2	-	-4*
1	28	-29
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-3	-	-4*
-4	40	-40
-5	32	-30
-6	20	19
-7	22	21
-8	-	3*
-9	29	-27
-10	35	-39

H 2 5

-10	16	13
-9	16	-15
-8	43	-44
-7	-	4*
-6	37	37
-5	43	43
-4	-	6*
-3	52	-53
-2	18	-18
-1	18	19
0	38	40
1	8	8
2	58	-58
3	39	-39
4	-	-7*
5	26	24
6	16	17
7	27	-28
8	23	-21
9	-	-4*

H 1 5

9	35	-36
8	10	7
7	18	16
6	31	32
5	14	10
4	40	-40
3	19	-17
2	31	30
1	55	56
0	23	27
-1	30	-33
-2	26	-27
-3	-	1*
-4	38	38
-5	35	36
-6	26	-28
-7	35	-36
-8	-	-7*
-9	19	20
-10	25	24

H 0 5

-10	13	-9
-9	22	22
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-7	-	7*
-6	-	1*
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1	13	-12
2	35	34
3	-	0*
4	28	-28
5	50	-49
6	25	-25
7	37	36
8	29	29
9	-	4*

H 13 6

0	23	23
-1	17	16

H 12 6

-4	-	14*
-3	-	-9*
-2	37	-37
-1	16	-14
0	10	8
1	14	12
2	-	4*
3	33	-30

H 11 6

4	-	-2*
3	22	22
2	39	40
1	22	22
0	26	-27
-1	29	-27
-2	-	-3*
-3	17	17
-4	12	12
-5	27	-25

H 10 6

-6	-	3*
-5	22	-21
-4	18	-17
-3	-	4*
-2	37	38
-1	10	8
0	22	-23
1	27	-26
2	11	-10
3	34	34
4	23	22
5	-	-6*

H 9 6

6	-	1*
5	34	34
4	20	19
3	-	-4*
2	20	-19
1	8	-8
0	28	28
-1	19	17
-2	-	-6*
-3	30	-30
-4	29	-30
-5	13	14
-6	16	17
-7	-	-4*

H 8 6

-8	-	-17*
-7	34	-35
-6	-	0*
-5	18	18
-4	20	17
-3	8	7
-2	34	-35
-1	10	-9
0	24	24
1	24	26
2	12	10
3	30	-32
4	16	-15
5	11	9
6	16	15
7	14	13

H 7 6

7	26	27
6	-	2*
5	36	-38
4	20	-19
3	13	12
2	30	31
1	16	14
0	34	-34
-1	26	-26
-2	-	1*
-3	32	33
-4	33	34
-5	20	-21
-6	28	-29
-7	-	-6*
-8	15	16

H 6 6

-8	14	8
-7	29	31
-6	-	-6*
-5	29	-28
-4	15	-15
-3	16	16
-2	65	65
-1	31	30
0	11	-8
1	17	-15
2	-	-2*
3	48	47
4	23	24
5	14	-15
6	30	-31
7	31	-29
8	18	15

H 5 6

8	16	-15
7	30	-28
6	-	-8*
5	24	24
4	-	4*
3	20	-19
2	38	-40
1	25	-25
0	33	34
-1	27	27
-2	-	-2*
-3	21	-21
-4	15	-14
-5	30	31
-6	33	33
-7	12	14
-8	17	-15
-9	27	-27

H 4 6

-9	-	6*
-8	11	-10
-7	44	-45
-6	14	-12
-5	22	23
-4	23	23
-3	-	0*
-2	37	-37
-1	-	0*
0	25	24
1	27	28
2	19	19
3	41	-39
4	23	-22
5	11	8
6	13	12
7	-	8*
8	30	-31

H 3 6

8	17	14
7	22	23
6	-	-6*
5	44	-44
4	23	-22
3	-	6*
2	31	31
1	18	19
0	41	-43
-1	31	-31
-2	13	10
-3	37	38
-4	35	36
-5	16	-13
-6	22	-20
-7	-	-5*
-8	23	24
-9	32	36

H 2 6

-9	-	-1*
-8	25	23
-7	45	46
-6	-	0*
-5	31	-31
-4	26	-26
-3	-	2*
-2	49	50
-1	7	5
0	33	-37
1	39	-41
2	20	-19
3	49	48
4	29	28
5	10	-8
6	19	-20
7	17	-18
8	32	30
9	29	29

H 1 6

9	-	1*
8	17	-17
7	30	-30
6	8	-7
5	36	36
4	16	13
3	21	-18
2	37	-37
1	19	-19
0	32	37
-1	24	27
-2	-	0*
-3	29	-30
-4	31	-31
-5	30	31
-6	36	35
-7	9	6
-8	17	-16
-9	24	-23
-10	-	9*

H 0 6

-10	30	33
-9	24	24
-8	-	-4*
-7	28	-29
-6	-	6*
-5	21	18
-4	14	13
-3	-	-7*
-2	66	-68
-1	40	-38
1	8	5
2	-	-4*
3	48	-47
4	16	-14
5	19	18
6	28	28
7	29	29
8	13	-15
9	12	-11

Reprinted from *Acta Crystallographica*, Vol. B 32, Part 9, September 1976

PRINTED IN DENMARK

Acta Cryst. (1976). B32, 2720

Ditellurium(IV) Trioxosulphate

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(*Received* 25 *March* 1976; *accepted* 10 *April* 1976)

Abstract. $Te_2O_3SO_4$, $P2_1nm$, orthorhombic, $a=4{\cdot}654$ (1), $b=6{\cdot}936$ (1), $c=8{\cdot}879$ (2) Å, $Z=2$, $V=286{\cdot}6$ (1) Å^3, $M=399{\cdot}26$, $D_x=4{\cdot}63$ g cm^{-3}. The S–O distances are 1·47 (1)–1·49 (1) Å. The Te^{IV} coordination is threefold pyramidal with Te–O distances of 1·89 (1), 1·91 (1) and 2·00 (1) Å. In addition there are three longer Te–O bonds of 2·26 (1), 2·63 (1) and 2·84 (1) Å. The TeO_3 and SO_4 units are connected to form sheets.

Introduction. The preparation of $Te_2O_3SO_4$ has been described by Hubková, Loub & Syneček (1966), who found that $Te_2O_3SO_4$ belonged to space group $P2_1nm$. Since there were, however, uncertainties about the proposed structure, a complete redetermination has been performed. Single crystals were prepared and provided by Dr Moret, Montpellier. The cell dimensions were refined (Lindqvist & Wengelin, 1967) from 48* lines measured on a Guinier powder photograph, taken with KCl as an internal standard ($a_{KCl}=6{\cdot}2919$ Å at 20°C; Hambling, 1953).

Intensities were collected on a two-circle Pailred diffractometer with Mo $K\alpha$ radiation and a graphite monochromator. The ω-scan procedure was used with a scan speed of 2·5° min^{-1} and the background was measured for 24 s at each end of the scan interval ($\Delta\omega=3$–6°). The layers $0kl$–$8kl$ were registered out to $2\theta=100°$ and 1050 unique reflexions for which $\sigma(I)/I<0{\cdot}3$ were used in the structure analysis. The intensities were corrected for absorption (program *DATAP2*; Coppens, Leiserowitz & Rabinovich, 1965). A drawing of the crystal used for the data collection is shown in Fig. 1. μ(Mo $K\alpha$) = 177·6 cm^{-1} (*International Tables for X-ray Crystallography*, 1962).

The structure was solved from Patterson and electron density calculations (program *DRF*; A. Zalkin, Berkeley) and the space group confirmed to be $P2_1nm$ in accordance with the systematic absences $h+l=2n+1$ for the $h0l$ reflexions. The structural parameters were refined with the block-diagonal approximation (program *BLOCK*; O. Lindgren, Göteborg), initially with isotropic temperature factors and separate scale factors for each layer ($R=0{\cdot}052$) and subsequently with anisotropic temperature factors and an overall scale factor ($R=0{\cdot}047$). The positional parameters obtained from

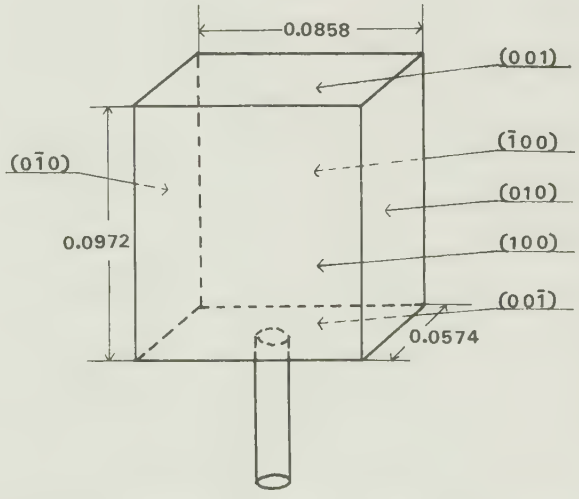

Fig. 1. The crystal used for data collection. The distances are given in mm.

* Lists of observed and calculated $\sin^2\theta_{hkl}$ and d_{hkl} values, and structure factors have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 31788 (8 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

the two refinements were the same within the standard deviations. The final parameters are given in Table 1. Scattering factors for Te (Cromer & Waber, 1965), S and O (Doyle & Turner, 1968) were corrected for the real part of the anomalous scattering (Cromer, 1965). Weights $w=20{\cdot}0+F_o+0{\cdot}004F_o^2$ were used. No extinction correction was performed, since only a few of the strongest reflexions appeared to be affected.

Discussion. Crystals of tellurates(IV) are usually prepared by hydrothermal syntheses or from melts. Action of conc. HNO_3 or H_2SO_4 on Te metal can also be used, *e.g.* TeO_2 (Lindqvist, 1968), $Te_2O_4.HNO_3$ (Swink & Carpenter, 1966) and $Te_2O_3SO_4$ (Hubková, Loub & Syneček, 1966). Both TeO_2 and $Te_2O_4.HNO_3$ have three-dimensional Te–O net structures with four-coordinated Te^{IV} atoms.

Bond distances and angles are given in Table 2. $Te_2O_3SO_4$ has a layer structure (Figs. 2 and 3) in which the SO_4 tetrahedron is strongly connected to the layers *via* two Te–O bonds of 2·26 (1) Å. The layers are held together by van der Waals contacts. A similar structural arrangement has been found in $Te_2O_3HPO_4$ (Mayer, 1975).

Table 1. *Atomic parameters in* $Te_2O_3SO_4$

Positional parameters are given as fractions of the lattice translation. The general point position in $P2_1nm$ is (x,y,z), $(x,y,-z)$, $(\frac{1}{2}+x,-y,\frac{1}{2}-z)$, $(\frac{1}{2}+x,-y,\frac{1}{2}+z)$. The isotropic temperature factor, B, is given in Å^2 and the anisotropic temperature factors correspond to the expression $T=\exp[-2\pi^2(U_{11}h^2a^{*2}+U_{22}k^2b^{*2}+U_{33}l^2c^{*2}+U_{12}hka^*b^*+U_{13}hla^*c^*+U_{23}klb^*c^*)\times 10^{-4}]$. Estimated standard deviations are given in parentheses.

	x	y	z	B	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Te	0†	0·1783 (1)	0·1991 (1)	0·458 (5)	57 (1)	67 (1)	49 (1)	13 (10)	−7 (9)	−5 (3)
S	0·4236 (9)	0·4809 (5)	0	0·57 (4)	69 (9)	72 (11)	72 (11)	−24 (21)	0	0
O(1)	0·657 (3)	0·338 (2)	0	1·1 (2)	115 (38)	205 (51)	126 (45)	268 (89)	0	0
O(2)	0·248 (2)	0·447 (1)	0·138 (1)	0·8 (1)	133 (28)	105 (26)	96 (27)	−17 (50)	133 (50)	−21 (49)
O(3)	0·088 (3)	0·091 (2)	0	0·6 (1)	106 (36)	70 (33)	50 (32)	−28 (66)	0	0
O(4)	0·635 (2)	0·091 (1)	0·263 (1)	1·1 (1)	84 (25)	116 (29)	257 (44)	−36 (57)	67 (68)	55 (66)
O(5)	0·029 (3)	0·318 (2)	0·5	1·3 (2)	152 (48)	175 (38)	174 (45)	328 (116)	0	0

† Fixed to specify origin along 2_1.

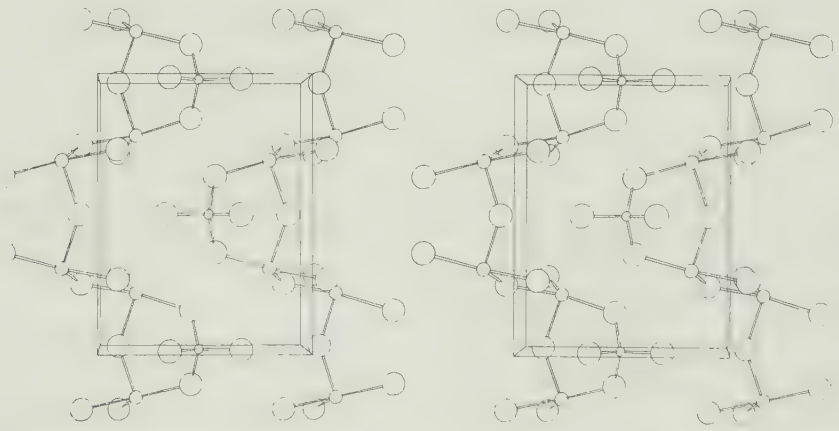

Fig. 2. A stereoscopic picture of the structure projected along the *c* axis (*ORTEP*; Johnson, 1965).

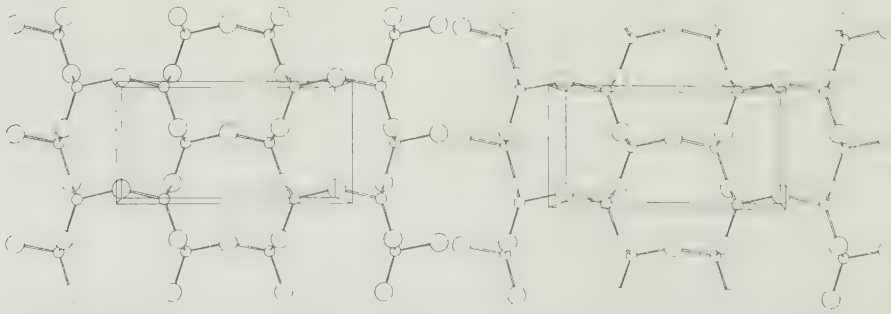

Fig. 3. A stereoscopic view along the *a* axis, showing one sheet of Te–O connexions (*ORTEP*; Johnson, 1965).

Table 2. *Distances and angles in* $Te_2O_3SO_4$

Te—O(4)	1·89 (1)	O(1)–Te–O(2)	78·5 (4)
–O(3)	1·914 (5)	O(1)———O(3)	69·1 (4)
–O′(4)	2·00 (1)	O(1)———O(4)	78·1 (4)
–O(2)	2·26 (1)	O(1)———O′(4)	134·3 (4)
–O(1)	2·63 (1)	O(1)———O(5)	121·1 (4)
–O(5)	2·844 (5)	O(2)———O(3)	86·0 (4)
–O(4)	3·07 (1)	O(2)———O(4)	142·8 (4)
S——O(1)	1·47 (1)	O(2)———O′(4)	130·5 (4)
–O(5)	1·48 (1)	O(2)———O(5)	85·5 (3)
–O(2) (2×)	1·49 (1)	O(3)———O(4)	111·6 (5)
		O(3)———O′(4)	77·9 (5)
O(1)–S–O(2)	107·3 (5)	O(3)———O(5)	164·9 (5)
O(2)–S–O(2)	110·5 (8)	O(4)———O′(4)	86·1 (3)
O(1)–S–O(5)	113·0 (8)	O(4)———O(5)	82·5 (4)
O(2)–S–O(5)	109·3 (5)	O′(4)——O(5)	98·4 (4)

The coordination of Te^{IV} is intermediate between three- and fourfold. Te^{IV} coordination can usually be described in terms of a trigonal bipyramid in which the two shortest Te^{IV}–O bonds are equatorial and the two next shortest are axial while the third equatorial position is occupied by a free electron pair (covalent type; Lindqvist, 1973). However, in $Te_2O_3SO_4$ three of the strongly coordinated O atoms lie in a plane [O(2), O(4) and O(4′)] while the fourth [O(3)] is perpendicular to this plane (Fig. 4). In addition there are two weak Te–O interactions (2·63 and 2·84 Å). The coordination may also be described in terms of an ionic model (Johansson & Lindqvist, 1976).

We thank Professor G. Lundgren for valuable discussions and Dr S. Jagner for revising the English text. Financial aid has been provided by the Swedish Natural Science Research Council (NFR, contract No. 2318).

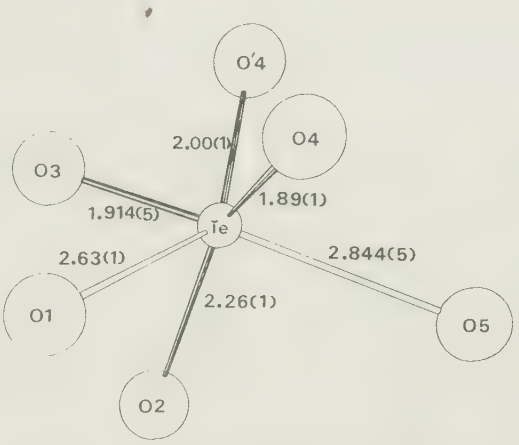

Fig. 4. The oxygen coordination of tellurium(IV).

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wder data for $Te_2O_3SO_4$
Kα, radiation (1.54050 Å)

H	K	L	SIN2TH OBS	SIN2TH CALC	DIFF	INT	D-OBS	D-CAL
0	1	0	12330	12332	-2	W	6.93665	6.9360
0	1	1	19770	19858	-88	M	5.47808	5.4659
0	0	2	29980	30104	-124	S	4.44852	4.4393
1	0	1	34760	34913	-153	VVW	4.13135	4.1222
1	1	0	39540	39720	-180	VS	3.87359	3.8648
0	1	2	42210	42437	-227	S	3.74907	3.7390
1	1	1	47050	47246	-196	M	3.55101	3.5436
0	2	0	49410	49330	80	VW	3.46517	3.4679
0	2	1	56780	56856	-76	VVW	3.23246	3.2303
1	1	2	69780	69824	-44	S	2.91586	2.9149
1	2	0	76660	76718	-58	M	2.78194	2.7808
0	2	2	79250	79434	-184	W	2.73610	2.7329
0	1	3	79920	80067	-147	M	2.72461	2.7221
1	2	1	84180	84244	-64	VW	2.65477	2.6537
1	0	3	94900	95122	-222	S	2.50034	2.4974
1	2	2	106730	106822	-92	W	2.35770	2.3566
1	1	3	107470	107455	15	VVW	2.34957	2.3497
2	0	0	109450	109549	-99	W	2.32822	2.3271
0	3	0	110870	110993	-123	W	2.31326	2.3119
0	2	3	116950	117065	-115	VW	2.25233	2.2512
2	1	0	121660	121882	-222	VW	2.20830	2.2062
2	1	1	129330	129408	-78	VVW	2.14181	2.1411
1	3	0	138190	138381	-191	VVW	2.07202	2.0705
2	0	2	139530	139654	-124	VVW	2.06204	2.0611
0	3	2	141050	141098	-48	M	2.05090	2.0505
1	2	3	144290	144452	-162	W	2.02775	2.0266
1	3	1	145710	145907	-197	VVW	2.01784	2.0164
2	1	2	151900	151986	-86	W	1.97630	1.9757
2	2	0	158560	158880	-320	W	1.93435	1.9324
1	1	4	160170	160137	33	VVW	1.92460	1.9248
2	2	1	166370	166406	-36	VVW	1.88840	1.8882
1	3	2	168660	168485	175	VVW	1.87554	1.8765
2	1	3	189480	189617	-137	M	1.76950	1.7688
1	2	4	197090	197135	-45	VVW	1.73500	1.7348
0	1	5	200240	200485	-245	M	1.72130	1.7202
1	3	3	205880	206116	-236	M	1.69756	1.6965
1	0	5	215420	215539	-119	W	1.65954	1.6590
2	3	0	220440	220543	-103	W	1.64054	1.6401
1	4	0	224550	224709	-159	W	1.62545	1.6248
2	2	3	226640	226615	25	VW	1.61794	1.6180
1	1	5	227690	227872	-182	W	1.61421	1.6135
2	0	4	229950	229967	-17	VVW	1.60626	1.6062
0	2	5	237370	237483	-113	VW	1.58095	1.5805
2	3	2	250540	250648	-108	VW	1.53884	1.5385
1	4	2	254620	254814	-194	W	1.52646	1.5258
3	1	0	258560	258819	-259	W	1.51478	1.5140
0	4	3	265000	265057	-57	M	1.49627	1.4961
3	1	2	288970	288924	46	W	1.43286	1.4329

Weight analysis according to Cruickshank (1970) and after the last cycle of refinement for $Te_2O_3SO_4$.

The quantities $w\Delta^2$ are normalized sums and N is the number of reflexions within each F_o interval.

F_o interval	N	$w\Delta^2$
0.0 - 15.7	105	2.643
15.7 - 19.1	105	1.154
19.1 - 22.4	105	1.123
22.4 - 26.7	105	0.909
26.7 - 31.5	105	0.501
31.5 - 37.1	105	0.340
37.1 - 42.8	105	0.478
42.8 - 51.6	105	0.510
51.6 - 70.4	105	0.480
70.4 - 138.5	106	1.860

Observed and calculated structure factors for $Te_2O_3SO_4$.

h	k	l	F_o	F_c	α
0	0	18	32	32	3.14
0	1	18	18	18	3.14
0	4	17	31	30	1.57
0	2	17	25	28	-1.57
0	1	17	32	31	-1.57
0	0	16	31	30	0.00
0	2	16	13	8	-3.14
0	3	16	23	22	3.14
0	6	16	16	18	0.00
0	7	15	44	46	1.57
0	5	15	23	26	-1.57
0	4	15	52	55	-1.57
0	2	15	45	42	1.57
0	1	15	54	54	1.57
0	0	14	31	29	0.00
0	3	14	19	19	3.14
0	9	13	25	27	1.57
0	8	13	23	22	-1.57
0	7	13	40	38	-1.57
0	6	13	21	24	-1.57
0	5	13	36	35	1.57
0	4	13	47	46	1.57
0	2	13	47	48	-1.57
0	1	13	50	50	-1.57
0	0	12	43	44	3.14
0	1	12	31	30	3.14
0	2	12	42	40	0.00
0	3	12	50	49	0.00
0	4	12	15	16	0.00
0	5	12	48	48	3.14
0	6	12	37	35	3.14
0	8	12	37	37	0.00
0	9	12	26	26	0.00
0	10	11	21	21	-1.57
0	7	11	18	21	1.57
0	5	11	13	15	-1.57
0	4	11	21	22	-1.57
0	2	11	30	27	1.57
0	1	11	30	29	1.57
0	0	10	100	101	0.00
0	1	10	31	29	0.00
0	2	10	52	50	3.14
0	3	10	83	83	3.14
0	5	10	49	47	0.00
0	6	10	71	73	0.00
0	8	10	46	46	3.14
0	9	10	44	44	3.14
0	10	10	16	13	0.00
0	11	10	35	35	0.00
0	10	9	22	19	-1.57
0	7	9	23	24	1.57
0	4	9	29	28	-1.57
0	2	9	18	15	1.57
0	1	9	27	24	1.57
0	0	8	52	52	3.14
0	1	8	58	55	3.14
0	2	8	75	71	0.00
0	3	8	73	71	0.00
0	4	8	24	22	0.00
0	5	8	76	73	3.14
0	6	8	57	54	3.14
0	8	8	46	46	0.00
0	9	8	44	41	0.00
0	11	8	34	34	3.14
0	12	8	21	18	3.14
0	13	7	21	22	-1.57
0	12	7	25	25	-1.57
0	10	7	34	34	1.57
0	9	7	36	34	1.57
0	8	7	40	38	-1.57
0	7	7	55	52	-1.57
0	6	7	41	40	-1.57
0	5	7	61	59	1.57
0	4	7	71	67	1.57
0	3	7	42	40	1.57
0	2	7	73	72	-1.57
0	1	7	76	73	-1.57
0	0	6	78	76	0.00
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0	2	6	13	15	-3.14
0	3	6	46	45	3.14
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0	10	5	65	64	-1.57
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0	6	5	38	36	1.57
0	5	5	64	62	-1.57
0	4	5	114	115	-1.57
0	3	5	23	23	-1.57
0	2	5	106	105	1.57
0	1	5	120	127	1.57
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0	3	4	39	36	3.14
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0	8	4	17	13	3.14
0	9	4	17	19	-3.14
0	10	4	17	14	0.00
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0	12	3	35	35	-1.57
0	11	3	16	17	1.57
0	10	3	39	39	1.57
0	9	3	41	41	1.57
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0	7	3	75	74	-1.57
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0	3	3	36	35	1.57
0	2	3	82	83	-1.57
0	1	3	110	119	-1.57
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0	4	2	40	39	0.00
0	5	2	86	88	3.14
0	6	2	56	54	-3.14
0	7	2	13	9	3.14
0	8	2	64	62	0.00
0	9	2	44	42	0.00
0	11	2	47	47	3.14
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0	14	2	27	27	0.00
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0	10	1	28	28	-1.57
0	7	1	39	38	1.57
0	4	1	57	56	-1.57
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0	1	0	51	51	0.00
0	2	0	60	63	3.14
0	3	0	138	169	3.14
0	4	0	35	33	3.14
0	5	0	59	60	0.00
0	6	0	97	97	0.00
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0	9	0	50	50	3.14
0	10	0	18	17	0.00
0	11	0	59	59	3.14
0	12	0	36	35	0.00
0	14	0	37	37	-3.14
1	0	17	37	39	3.14
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1	4	16	16	16	-1.42
1	2	16	20	16	1.58
1	1	16	19	18	1.57
1	0	15	50	49	0.08
1	1	15	31	31	-0.18
1	2	15	39	39	3.00
1	3	15	47	50	-3.03
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1	6	15	37	37	0.00
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1	5	13	38	34	-3.03
1	6	13	50	49	-3.11
1	8	13	34	34	0.02
1	9	13	28	28	-0.02
1	10	12	33	33	1.51
1	7	12	44	46	-1.58
1	6	12	17	15	-1.53
1	5	12	27	26	1.58
1	4	12	53	53	1.56
1	2	12	42	41	-1.62
1	1	12	51	51	-1.54
1	0	11	18	17	-0.27
1	1	11	26	23	0.05
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1	3	11	23	22	-2.98
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1	6	11	16	14	0.26
1	8	11	21	20	2.90
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1	11	11	16	15	-0.18
1	10	10	42	42	-1.48
1	9	10	39	39	-1.57
1	8	10	27	28	1.47
1	7	10	53	56	1.54
1	6	10	31	31	1.57
1	5	10	48	49	-1.59
1	4	10	68	68	-1.61
1	3	10	18	18	-1.60
1	2	10	75	72	1.66
1	1	10	82	80	1.56
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1	4	9	18	16	2.89
1	5	9	22	23	-0.28
1	8	9	18	16	3.00
1	11	9	16	15	0.09
1	12	8	21	22	-1.52
1	10	8	48	47	1.53
1	9	8	24	23	1.74
1	8	8	15	17	-1.43
1	7	8	63	63	-1.66
1	6	8	24	24	-1.26
1	5	8	42	39	1.79
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1	3	8	17	14	1.95
1	2	8	67	65	-1.50
1	1	8	83	79	-1.56
1	0	7	112	111	3.05
1	1	7	24	27	-2.58
1	2	7	52	49	0.32
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1	4	7	15	13	0.80
1	5	7	48	43	-3.10
1	6	7	71	69	-3.13
1	8	7	45	44	-0.03
1	9	7	41	39	0.00
1	11	7	33	34	3.09
1	12	7	21	22	-3.06
1	10	6	16	15	-1.26
1	9	6	25	24	-1.54
1	7	6	17	17	1.64
1	6	6	17	18	1.14
1	5	6	28	27	-1.98
1	4	6	23	21	-1.40
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1	2	5	89	87	3.04
1	3	5	117	117	-3.05
1	4	5	42	40	3.03
1	5	5	90	88	-0.09
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1	11	5	53	54	0.01
1	12	5	28	29	0.04
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1	9	4	16	19	-1.77
1	8	4	20	18	1.67
1	7	4	23	19	1.58
1	6	4	21	17	1.74
1	5	4	28	28	-1.44
1	4	4	31	26	-1.62
1	3	4	21	23	-0.89
1	2	4	44	32	1.76
1	1	4	43	40	1.23
1	0	3	134	165	-3.03
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1	2	3	74	70	0.02
1	3	3	114	114	-0.07
1	4	3	16	13	0.55
1	5	3	62	59	-3.04
1	6	3	91	89	3.10
1	8	3	56	54	0.14
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1	10	3	16	13	2.69
1	11	3	39	38	-3.07
1	12	3	25	25	3.07
1	13	3	17	14	0.02
1	13	2	24	31	-1.74
1	12	2	23	24	-1.49
1	10	2	53	53	1.45
1	9	2	24	21	1.51
1	8	2	29	27	-1.30
1	7	2	85	84	-1.54
1	6	2	32	32	-1.39
1	5	2	56	55	1.71
1	4	2	120	123	1.62
1	3	2	41	39	2.02
1	2	2	78	82	-1.88
1	1	2	99	107	-1.63
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1	3	1	53	51	-2.63
1	4	1	29	27	2.74
1	5	1	42	41	-0.17
1	8	1	26	25	-3.13
1	9	1	15	15	-3.14
1	11	1	21	22	0.13
1	13	0	26	33	1.53
1	12	0	38	41	1.55
1	11	0	21	18	-1.70
1	10	0	53	53	-1.54
1	9	0	50	51	-1.67
1	8	0	51	45	1.50
1	7	0	90	87	1.69
1	6	0	56	52	1.35
1	5	0	87	85	-1.77
1	4	0	117	126	-1.36
1	3	0	62	47	-1.76
1	2	0	113	130	1.41
1	1	0	127	163	1.55
2	1	17	30	30	-1.58
2	2	17	24	26	-1.56
2	4	17	26	26	1.61
2	6	16	15	16	-0.13
2	1	15	46	47	1.60
2	2	15	41	44	1.61
2	4	15	44	48	-1.64
2	5	15	29	30	-1.51
2	6	15	17	19	1.68
2	7	15	38	39	1.49
2	3	14	17	16	2.68
2	0	14	16	16	-0.26
2	1	13	48	50	-1.56
2	2	13	39	40	-1.57
2	4	13	44	47	1.65
2	5	13	32	32	1.43
2	6	13	22	21	-1.74
2	7	13	39	41	-1.51
2	8	13	21	19	-1.77
2	9	13	23	23	1.48
2	9	12	29	27	0.10
2	8	12	31	32	-0.10
2	6	12	37	38	-3.05
2	5	12	41	40	3.10
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6	6	10	37	37	-0.06
6	5	10	41	40	0.01
6	3	10	41	44	3.11
6	2	10	39	38	-3.12
6	1	10	26	25	0.06
6	0	10	50	51	0.02
6	5	9	15	14	-1.71
6	8	8	32	28	0.01
6	6	8	36	38	3.09
6	5	8	27	30	3.07
6	3	8	55	56	0.04
6	2	8	21	20	-0.08
6	1	8	14	14	-3.01
6	0	8	57	58	-3.08
6	1	7	45	46	-1.51
6	2	7	37	35	-1.60
6	4	7	49	50	1.52
6	5	7	21	19	1.50
6	7	7	42	42	-1.53
6	9	7	18	16	1.70
6	8	6	19	16	-3.07
6	6	6	15	16	-0.12
6	5	6	21	21	-0.03
6	2	6	26	25	-3.06
6	1	6	17	16	0.31
6	1	5	59	59	1.54
6	2	5	49	48	1.64
6	3	5	19	17	-1.52
6	4	5	58	59	-1.57
6	5	5	42	42	-1.59
6	6	5	27	29	1.71
6	7	5	50	50	1.47
6	8	5	25	24	1.58
6	9	5	27	25	-1.50
6	10	5	34	31	-1.55
6	8	4	20	19	3.13
6	5	4	17	19	0.26
6	2	4	21	19	-2.91
6	1	4	14	12	-0.18
6	0	4	18	20	-0.37
6	1	3	52	52	-1.50
6	2	3	49	48	-1.60
6	4	3	51	51	1.53
6	5	3	28	28	1.54
6	6	3	14	16	-1.68
6	7	3	45	45	-1.49
6	8	3	17	16	-1.88
6	9	3	20	21	1.67
6	10	3	36	36	1.55
6	9	2	31	31	0.04
6	8	2	30	31	-0.01
6	6	2	43	42	-3.08
6	5	2	32	31	-3.05
6	3	2	64	64	0.03
6	2	2	24	24	-0.01
6	1	2	22	23	2.90
6	0	2	67	68	3.09
6	1	1	19	18	1.43
6	2	1	18	18	1.72
6	3	1	11	11	-1.53
6	4	1	14	16	-1.43
6	5	1	23	22	-1.60
6	6	1	16	17	1.74
6	9	0	36	36	3.11
6	8	0	44	47	-3.12
6	6	0	52	51	0.06
6	5	0	53	54	0.12
6	4	0	25	24	3.06
6	3	0	54	54	3.07
6	2	0	57	59	-3.06
6	1	0	41	44	-0.08
7	0	13	28	28	-3.00
7	4	12	24	24	1.54
7	2	12	24	26	-1.58
7	1	12	27	28	-1.61
7	0	11	17	17	0.04
7	3	11	18	19	-3.00
7	5	10	21	21	-1.67
7	4	10	42	41	-1.52
7	2	10	34	35	1.49
7	1	10	40	41	1.57
7	0	9	15	17	-0.29
7	3	9	16	17	3.11
7	6	9	16	11	-0.22
7	7	8	28	28	-1.53
7	5	8	23	25	1.46
7	4	8	32	34	1.68
7	2	8	35	35	-1.62
7	1	8	38	40	-1.55
7	0	7	39	41	-2.98
7	1	7	26	26	2.95
7	2	7	31	31	-0.10
7	3	7	31	33	0.00
7	4	7	14	15	-0.08
7	5	7	27	28	3.08
7	6	7	26	26	-3.14
7	8	7	27	30	0.08
7	7	6	18	16	1.68
7	4	6	18	19	-1.59
7	2	6	15	15	1.54
7	1	6	20	18	1.53
7	0	5	62	63	-0.06
7	1	5	23	18	0.02
7	2	5	29	26	-3.12
7	3	5	61	61	-3.12
7	5	5	34	36	0.11
7	6	5	43	44	-0.07
7	8	5	31	31	-3.09
7	9	5	30	30	3.12
7	7	4	19	18	1.67
7	4	4	22	22	-1.52
7	3	4	14	6	-1.80
7	1	4	14	13	1.66
7	0	3	45	46	-3.09
7	1	3	31	30	-3.12
7	2	3	39	37	0.05
7	3	3	37	38	-0.06
7	4	3	19	17	0.02
7	5	3	35	34	3.07
7	6	3	32	32	-3.05
7	8	3	33	34	-0.02
7	9	3	21	21	-0.01
7	10	2	25	23	1.68
7	9	2	20	20	1.59
7	8	2	20	19	-1.79
7	7	2	35	35	-1.65
7	6	2	22	22	-1.49
7	5	2	30	32	1.53
7	4	2	42	42	1.55
7	3	2	14	14	1.40
7	2	2	36	36	-1.51
7	1	2	41	42	-1.55
7	0	1	23	24	-0.33
7	1	1	8	4	1.28
7	2	1	11	5	-2.48
7	3	1	27	26	3.14
7	4	1	14	2	0.41
7	5	1	18	12	0.31
7	6	1	18	18	-0.09
7	7	1	12	4	2.77
7	8	1	14	7	3.00
7	9	1	17	12	-2.95
7	10	0	37	38	-1.64
7	9	0	22	18	-1.34
7	8	0	23	21	1.58
7	7	0	52	52	1.55
7	6	0	21	19	1.72
7	5	0	35	30	-1.49
7	4	0	62	62	-1.64
7	3	0	21	17	-1.27
7	2	0	42	42	1.62
7	1	0	47	52	1.56
8	3	8	36	34	0.01
8	2	8	21	19	0.09
8	0	8	36	35	3.04
8	1	7	31	30	-1.60
8	2	7	25	26	-1.56
8	4	7	31	30	1.53
8	2	6	13	14	3.09
8	0	6	16	11	0.40
8	0	5	13	0	1.58
8	1	5	42	41	1.56
8	2	5	39	37	1.47
8	3	5	14	13	-1.49
8	4	5	38	40	-1.48
8	5	5	28	29	-1.64
8	6	5	17	20	1.59
8	2	4	18	14	2.96
8	1	4	19	16	-0.34
8	0	4	15	12	0.54
8	1	3	38	38	-1.57
8	2	3	30	29	-1.51
8	3	3	14	6	1.84
8	4	3	42	40	1.53
8	5	3	17	18	1.57
8	6	2	29	30	2.87
8	5	2	22	23	-3.04
8	4	2	14	9	0.30
8	3	2	43	43	-0.01
8	2	2	20	18	0.04
8	1	2	16	17	-2.71
8	0	2	45	49	3.08
8	2	1	13	12	1.36
8	3	1	12	4	-1.40
8	4	1	18	14	-1.39
8	6	0	31	31	0.13
8	5	0	33	34	-0.10
8	4	0	19	14	2.93
8	3	0	44	46	-3.14
8	2	0	31	33	3.10
8	1	0	20	27	-0.18

Acta Cryst. (1977). B33, 2418–2421

The Crystal Structure of Amminecopper(II) Tellurate(IV) Monohydrate $Cu(NH_3)TeO_3.H_2O$

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(*Received* 23 *December* 1976; *accepted* 28 *January* 1977)

Single crystals of $Cu(NH_3)TeO_3.H_2O$ have been prepared by hydrothermal synthesis. The space group is $C2/c$ with $a = 12{\cdot}988$ (4), $b = 7{\cdot}333$ (1), $c = 10{\cdot}022$ (3) Å, $\beta = 97{\cdot}18$ (3)°. The structure parameters were refined to an R of 0·040 with 1283 independent reflexions. The structure contains pyramidal TeO_3^{2-} ions with Te–O distances of 1·867–1·881 Å. The Cu^{II} coordination is square planar with three O atoms at 1·947–1·958 Å, while the fourth corner is occupied by an ammonia molecule with Cu–N = 1·993 Å. The Te and Cu atoms share O atoms thus forming a layer structure. The water of crystallization is situated between the layers.

Introduction

Previous structure investigations of Cu^{II} tellurates(IV) comprise $CuTeO_3.2H_2O$ (Zemann & Zemann, 1962), $CuTeO_3$ (Lindqvist, 1972) and $CuTe_2O_5$ (Hanke, Kupčik & Lindqvist, 1973).

$CuTeO_3$ and $CuTe_2O_5$ were both prepared from CuO–TeO_2 melts, and the crystals had complicated three-dimensional network structures. The strong covalent connexions result in irregular Te and Cu polyhedra. In the mineral teinite ($CuTeO_3.2H_2O$), on the other hand, the presence of water of crystallization permits a more regular arrangement of O around the metal atoms, *i.e.* threefold pyramidal for Te^{IV} and square planar for Cu^{II}.

The Cu^{II} tellurate(IV) crystals used in this study were prepared by Dr Jacques Moret, Montpellier, by hydrothermal synthesis from CuO and TeO_2 in NH_3(aq.). The crystals were suspected to contain both water and ammonia molecules.

Experimental

Unit-cell dimensions and space-group extinctions were investigated with a Weissenberg camera. Accurate cell dimensions (Table 1) were obtained from a Guiner powder film exposed with KCl as internal standard. The cell constants were refined by least squares based on 41 $\sin^2\theta$ values (*POWDER*; Lindqvist & Wengelin, 1967).*

* Lists of structure factors, anisotropic thermal parameters and Guinier powder data have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 32482 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

The crystal used for data collection was mounted along **b** (Fig. 1) on a two-circle Pailred diffractometer. Mo $K\alpha$ radiation, monochromated with a graphite crystal, was used. The reflexions were measured with the ω-scan technique and a scan speed of 2·5° min^{-1} over scan intervals in the range 3·0–6·0°, depending on μ and 2θ. The background was measured for 24 s at each end of the scan interval. The $h0l$–$h,10,l$ reflexions

Table 1. *Crystallographic data for* $Cu(NH_3)TeO_3.H_2O$

a 12·988 (4) Å	Formula weight	274·2
b 7·333 (1)	Density D_x	3·87 g cm^{-3}
c 10·022 (3)	Space group	$C2/c$ or Cc
β 97·18 (3)°	Absorption coefficient	97·5 cm^{-1}
V 942·2 $Å^3$	μ(Mo $K\alpha$)	
Z 8	Crystal habit	Blue plates

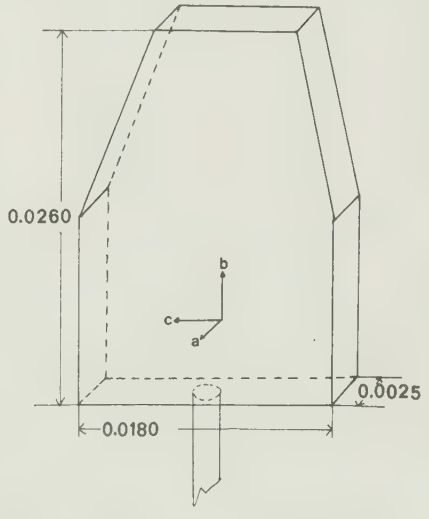

Fig. 1. The crystal used in data collection.

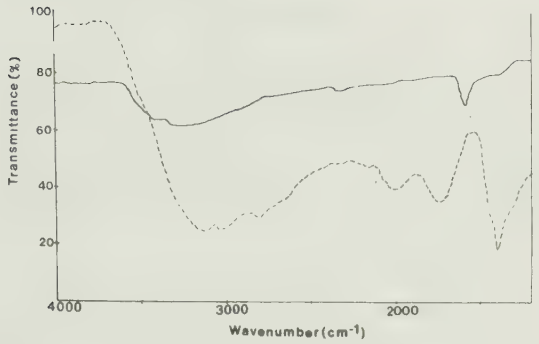

Fig. 2. IR spectra of $Cu(NH_3)TeO_3.H_2O$ (full curve) and NH_4Cl (dotted curve).

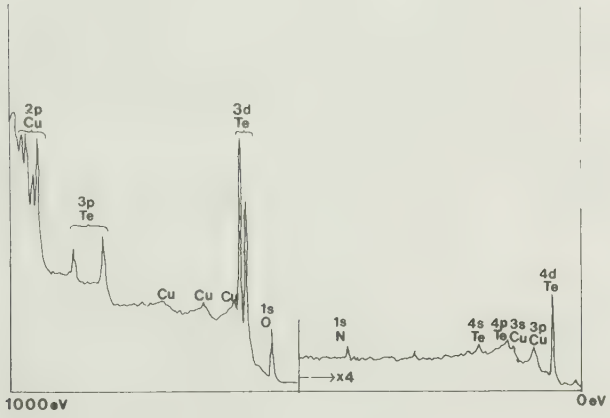

Fig. 3. ESCA spectrum of $Cu(NH_3)TeO_3.H_2O$.

with $2\theta < 70°$ were registered, and 1283 intensities with $\sigma(I)/I < 0{\cdot}2$ were regarded as significant. Corrections for Lorentz and polarization effects were performed with the program *DATAP*1 (O. Lindgren, Göteborg).

At the commencement of the X-ray study, the structural roles of the water and ammonia molecules were not obvious. To confirm the X-ray investigation, spectroscopic and thermogravimetric measurements were also made. The IR spectrum (Fig. 2) was obtained with a Perkin–Elmer 337 spectrophotometer with KBr as internal standard. The chemical analysis was carried out with a Hewlett–Packard ESCA apparatus. The heights of the O(1*s*) and N(1*s*) peaks (Fig. 3) indicated a N:O atomic ratio of 1:4.

Determination of the structure

The Te atoms were found to occupy the general position 8(*f*) from the Patterson function, and the other non-hydrogen atoms were located from successive electron density calculations. The Fourier summations were carried out with the program *FFT* (Ten Eyck, 1973). A preliminary least-squares refinement gave an R of 0·11. It was, however, apparent that the reflexions suffered from absorption. After a correction had been performed (*DATAP*2; Coppens, Leiserowitz & Rabinovich, 1965), R dropped to 0·05. No significant extinction effects were present.

The least-squares refinement was carried out with the block-diagonal approximation program *BLOCK* (O. Lindgren, Göteborg). In the final cycles, the refinement was extended to include anisotropic temperature factors, and the resulting positional parameters are given in Table 2.* Scattering factors for Te were obtained from Cromer & Waber (1965), while those given by Doyle & Turner (1968) were used for Cu, O and N. The observations were weighted according to $w = (20{\cdot}0 + F_o + 0{\cdot}004F_o^2)^{-1}$. Interatomic bond distances and angles (Tables 3 and 4) were calculated with the program *DISTAN* (A. Zalkin, Berkeley).

According to the ESCA results and the atomic positions obtained, the chemical formula might be either $NH_4Cu(OH)TeO_3$ or $Cu(NH_3)TeO_3.H_2O$.

* See previous footnote.

Table 2. *Positional parameters for* $Cu(NH_3)TeO_3.H_2O$

Standard deviations are given in parentheses.

	x	*y*	*z*
Te	0·24441 (4)	0·21261 (7)	0·31340 (5)
Cu	0·3332 (1)	0·0941 (1)	0·0302 (1)
N	0·4396 (7)	0·2660 (13)	−0·0244 (8)
O(1)	0·3044 (6)	0·2823 (9)	0·1594 (7)
O(2)	0·3604 (5)	−0·0872 (9)	−0·1036 (7)
O(3)	0·2298 (5)	−0·0636 (9)	0·0977 (7)
O(4)	$\frac{1}{2}$	0·0454 (20)	$\frac{3}{4}$
O(5)	$\frac{1}{2}$	0·4740 (20)	$\frac{1}{4}$

Table 3. *Coordination distances* (Å) *and angles* (°) *around* Te^{IV} *and* Cu^{II}

Te–O(2)	1·870 (7)	Cu–O(2)	1·950 (8)
Te–O(3)	1·877 (7)	Cu–O(3)	1·958 (7)
Te–O(1)	1·885 (8)	Cu–O(1)	1·960 (9)
Te–O(3′)	2·950 (7)	Cu–N	1·998 (7)
Te–O(3″)	3·082 (7)	Cu–O(1′)	2·602 (9)
Te–O(1′)	3·236 (9)	Cu–O(4)	3·066 (6)
O(1)–Te–O(2)	96·1 (4)	N–Cu–O(1)	86·1 (3)
O(1)–Te–O(3)	94·7 (3)	N–Cu–O(2)	92·9 (3)
O(2)–Te–O(3)	97·6 (3)	N–Cu–O(3)	175·3 (3)
O(1)–Te–O(1′)	116·1 (3)	O(1)–Cu–O(2)	178·0 (4)
O(1)–Te–O(3′)	65·3 (3)	O(1)–Cu–O(3)	89·5 (3)
O(1)–Te–O(3″)	159·1 (3)	O(2)–Cu–O(3)	91·5 (3)
O(1′)–Te–O(2)	68·8 (3)	N–Cu–O(1′)	90·9 (3)
O(1′)–Te–O(3)	146·9 (3)	N–Cu–O(4)	87·5 (3)
O(1′)–Te–O(3′)	52·9 (2)	O(1)–Cu–O(1′)	93·8 (3)
O(1′)–Te–O(3″)	62·7 (2)	O(1)–Cu–O(4)	86·4 (4)
O(2)–Te–O(3′)	87·9 (3)	O(1)–Cu–O(2)	84·4 (4)
O(2)–Te–O(3″)	63·4 (3)	O(1)–Cu–O(3)	91·1 (3)
O(3)–Te–O(3′)	159·8 (2)	O(1)–Cu–O(4)	178·4 (3)
O(3)–Te–O(3′)	84·3 (3)	O(2)–Cu–O(4)	95·4 (3)
O(3)–Ye–O(3″)	115·4 (1)	O(3)–Cu–O(4)	90·5 (3)

Table 4. *Distances* (Å) *and angles* (°) *for possible hydrogen bonding*

N–O(4)	2·96 (1)	Cu–N–O(4)	97·1 (4)
N–O(2)	3·05 (1)	Cu–N–O(2)	101·3 (3)
N–O(3)	3·12 (1)	Cu–N–O(3)	90·8 (3)
N–O(5)	3·16 (1)	Cu–N–O(5)	99·8 (3)
N′–O(5)	3·13 (1)	Cu–N′–O(5)	145·8 (3)
2× O(4)–O(2)	2·66 (1)	N–O(4)–N	113·9 (6)
		N–O(4)–O(2)	60·9 (2)
		N–O(4)–O(2)	152·3 (4)
		O(2)–O(4)–O(2)	137·0 (8)
2× O(5)–O(1)	2·95 (1)	N–O(5)–N	122·3 (5)
		N–O(5)–N′	73·9 (2)
		N–O(5)–N′	150·0 (3)
		N′–O(5)–N′	104·9 (5)
		N–O(5)–O(1)	52·4 (3)
		N–O(5)–O(1)	98·6 (4)
		N′–O(5)–O(1)	110·6 (2)
		N′–O(5)–O(1)	103·2 (2)
		O(1)–O(5)–O(1)	123·1 (6)

However, the colour of the crystals, which are bright blue instead of green, like $CuTeO_3$, $CuTe_2O_5$ and $Cu(OH)IO_3$ (*Handbook of Chemistry and Physics*, 1968), and the IR spectrum (Fig. 2), suggest that the formula is $Cu(NH_3)TeO_3.H_2O$.

As indicated in Table 2, O(4) and O(5) occupy special positions in *C*2/*c*, on twofold axes. Since, both O(4) and O(5) correspond to water of crystallization, they could not possibly occupy these positions in a fully ordered structure. The structure was therefore also refined in *Cc*, but no significantly different results were obtained. Neither did a difference synthesis based on the *C*2/*c* model show any anomalies. The highest peaks, corresponding to 1·3 e $Å^{-3}$, occurred near the heavy-atom positions. We therefore decided to describe the structure as belonging to *C*2/*c* with the exception of the water H atoms, which may be arranged in a disordered way, or in accordance with *Cc* symmetry.

Discussion

The structure is built up from TeO_3 pyramids bonded *via* O bridges to three Cu atoms. The Cu^{II} coordination is square planar with three corners of the square occupied by O atoms from different TeO_3 groups and the fourth by an ammonia molecule. This arrangement results in infinite sheets (Fig. 4) separated by water of crystallization (Fig. 5).

The Cu^{II} coordination distances are normal (Table 3). The Cu–O distances are very close to those found in $CuTe_2O_5$ (Hanke, Kupčik & Lindqvist, 1973) in which they range from 1·950 (3) to 1·969 (3) Å. The Cu–N distance of 1·997 (7) Å falls well within the range 1·97–2·07 Å observed in other ammine Cu^{II} complexes (Meyer, Singh, Hatfield & Hodgson, 1972). The deviations from the planar configuration of 0·03 Å in tetrahedral directions (Table 5) are significant. In addition to the four planar bonds, there are two longer Cu–O interactions of 2·602 (7) and 3·066 (7) Å completing a distorted octahedron.

In the ideal case of Te^{IV}–O threefold coordination, the TeO_3^{2-} ion ought to possess a threefold axis through the inert Te 5*s* electron pair and the centre of the Te atom. The bond distances and angles in $Cu(NH_3)TeO_3.H_2O$ (Table 3) correspond well to this geometry: three Te–O distances not significantly different from the mean value of 1·880 Å, and angles slightly different from the mean value of 96·15°. In $BaTeO_3.H_2O$ (Nielsen, Hazell & Rasmussen, 1971), which is evidently ionic, the corresponding bond distances are 1·847–1·859 (6) Å and the angles are 96·5–102·7 (3)°, with average values of 1·855 Å and 99·32°. Neither $BaTeO_3.H_2O$ nor $Cu(NH_3)TeO_3.H_2O$ contain any significant 'backbonding', *i.e.* one to three weak bonds opposite to the pyramidal Te–O bonds. This also supports the presence of TeO_3^{2-} ions in the two structures.

There are several N···O and O···O distances in $Cu(NH_3)TeO_3.H_2O$ which could be consistent with hydrogen bonding (Table 4). With respect to the angles around N, the N–O(2), N–O(4) and N–O(5) dis-

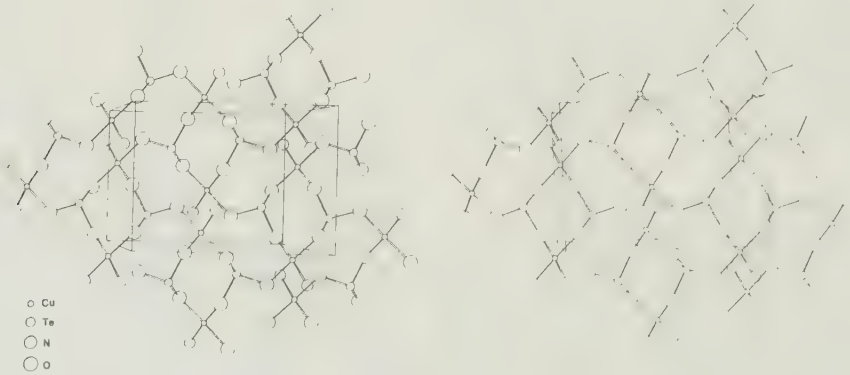

Fig. 4. A stereoscopic drawing of one $Cu(NH_3)TeO_3$ layer (*ORTEP*, Johnson, 1965).

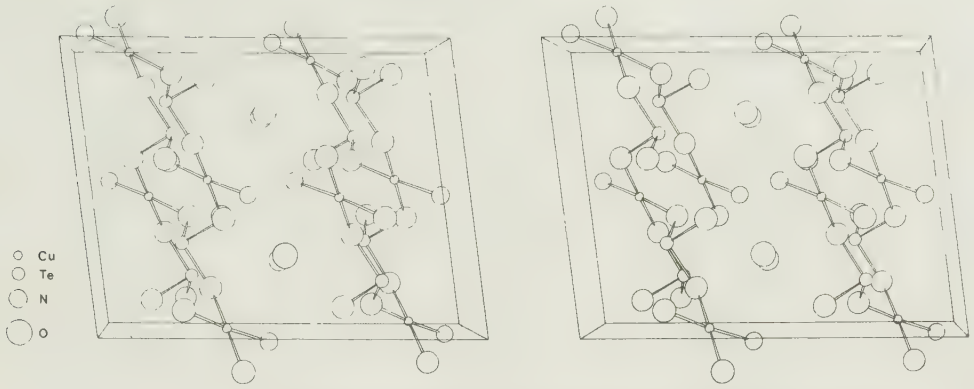

Fig. 5. The $Cu(NH_3)TeO_3.H_2O$ structure seen along the layers (*ORTEP*, Johnson, 1965).

Table 5. *Deviations* (Δ) *from a least-squares plane through the* Cu *planar coordination*

	Δ (Å)		Δ (Å)
Cu	0·000	O(2)	0·029
N	−0·030	O(3)	−0·030
O(1)	0·031		

tances of 3·045, 2·963 and 3·156 Å respectively, ought to correspond to N–H···O hydrogen bonds. Since the H atoms attached to the water molecules do not conform to the *C*2/*c* structure, no definite conclusions can be drawn concerning the O–H···O (or O–H···N) hydrogen bonds. However, it is possible that the true space group is *Cc* with all but the water H atoms being in agreement with *C*2/*c* symmetry. In this case, the water molecules could be hydrogen bonded according to O(1)···H–O(5)–H···O(1) and O(2)···H–O(4)–H···O(2) (Table 4).

We thank Professor Georg Lundgren for his support of this work, Dr Susan Jagner for revising the English text, and Dr John Wood for helping us to interpret the ESCA spectrum. Financial aid has been provided by the Swedish Natural Science Research Council (NFR: contract No. 2318).

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Guinier powder data for $Cu(NH_3)TeO_3 \cdot H_2O$

hkl	I obs	$10^5 \sin^2\theta$ obs	$10^5 \sin^2\theta$ calc	d Å calc
200	vs	1414	1429	6.443
110	vw	1472	1461	6.374
111	vw	2175	2176	5.221
002	vw	2402	2200	4.972
112	vw	4096	4092	3.808
202	w	4292	4292	3.718
020	w	4399	4413	3.667
021	M	5009	5013	3.440
311	M	5252	5266	3.356
400	M	5702	5717	3.221
220	s	5836	5842	3.187
221	w	6666	6674	2.982
022	w	6801	6813	2.951
113	M	7203	7208	2.869
312	vw	7422	7414	2.829
222	vs	8692	8705	2.611
402	w	9029	9043	2.561
510	vw	10021	10036	2.431
420	w	10104	10130	2.420
313	w	10755	10761	2.348
131	vw	10996	11002	2.322
421	vw	11189	11193	2.302
114	vw	11511	11524	2.269
600	vw	12853	12863	2.148
422	vw	13433	13456	2.100
331	vw	14101	14092	2.051
314	vw	15293	15309	1.969
133	vw	16007	16034	1.924
602	vw	16651	16652	1.888
115	vw	17025	17040	1.866
620	vw	17275	17276	1.853
205	vw	17584	17588	1.837
041	vw	18251	18252	1.803
025	vw	19411	19414	1.748
333	vw	19585	19587	1.740
042	vw	20059	20052	1.720
134	vw	20340	20350	1.707
315	w	21045	21056	1.679
006	vw	21609	21602	1.657
242	vw	21930	21944	1.644
532	vw	22424	22420	1.627

The anisotropic thermal parameters for $Cu(NH_3)TeO_3 \cdot H_2O$.

The anisotropic temperature factor is of the form

$$\exp[-2\pi^2 (h^2a^{*2} U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2hka^*b^*U_{12} + 2hla^*c^*U_{13} + 2klb^*c^*U_{23})] \cdot 10^3.$$

Standard deviations are given in parantheses.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Te	11.1(1)	12.6(2)	13.6(2)	0.4(4)	5.7(3)	-0.8(3)
Cu	15.3(4)	11.6(4)	12.7(4)	-4.7(8)	10.6(7)	-2.4(7)
N	21(2)	24(2)	19(3)	-22(4)	12(5)	-9(5)
O(1)	22(3)	11(3)	25(3)	1(6)	22(5)	-5(6)
O(2)	10(2)	22(3)	17(3)	-11(4)	7(4)	-12(5)
O(3)	17(2)	19(3)	16(2)	4(4)	18(4)	14(5)
O(4)	124(5)	32(6)	125(7)	-	233(39)	-
O(5)	38(6)	30(6)	63(9)	-	4(13)	-

Observed and calculated structure factors for $Cu(NH_3)TeO_3.H_2O$

h	k	l	F_o	F_c
-2	0	16	709	-597
-12	0	14	1473	-1400
-10	0	14	1423	1418
-8	0	14	939	-958
-6	0	14	489	478
-4	0	14	367	-367
-2	0	14	933	927
0	0	14	1407	-1357
2	0	14	1116	1071
4	0	14	657	-639
-4	0	12	1003	966
-6	0	12	699	-661
-14	0	12	659	-646
-16	0	10	573	563
-14	0	10	700	-693
-8	0	10	341	339
-6	0	10	1126	-1123
-4	0	10	1750	1775
-2	0	10	1566	-1608
0	0	10	917	986
2	0	10	549	-601
4	0	10	613	591
6	0	10	1533	-1457
8	0	10	1729	1717
10	0	10	1359	-1385
12	0	10	810	795
16	0	8	1011	-984
14	0	8	1419	1340
12	0	8	1140	-1117
10	0	8	862	885
8	0	8	891	-917
6	0	8	1721	1787
4	0	8	3054	-3112
2	0	8	3172	3196
0	0	8	1860	-1830
-2	0	8	943	958
-4	0	8	529	-575
-6	0	8	1987	2019
-8	0	8	2306	-2327
-10	0	8	2050	2024
-12	0	8	1236	-1197
-14	0	8	686	656
-16	0	8	575	-513
-18	0	8	880	801
-20	0	6	693	722
-18	0	6	966	-939
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-14	0	6	2359	-2387
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-10	0	6	1305	-1324
-6	0	6	1392	-1383
-4	0	6	2931	2975
-2	0	6	3503	-3609
0	0	6	2263	2307
2	0	6	826	-843
6	0	6	907	-953
8	0	6	1164	1117
10	0	6	1178	-1209
12	0	6	774	697
14	0	4	451	-490
12	0	4	1441	1391
10	0	4	1579	-1499
8	0	4	783	743
4	0	4	721	-697
2	0	4	705	678
0	0	4	928	898
-2	0	4	476	325
-6	0	4	2090	2154
-8	0	4	2161	-2186
-10	0	4	1242	1253
-18	0	4	1174	1226
-20	0	4	1009	-1054
-18	0	2	666	713
-12	0	2	390	-319
-10	0	2	784	716
-8	0	2	2494	-2494
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-4	0	2	2423	-2577
-2	0	2	1003	938
0	0	2	529	-633
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4	0	2	4187	-4457
6	0	2	3578	3630
8	0	2	2629	-2539
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12	0	2	580	-589
14	0	2	1238	1285
16	0	2	1524	-1625
18	0	2	1342	1430
20	0	2	877	-910
20	0	0	553	580
16	0	0	951	990
14	0	0	1520	-1558
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10	0	0	2786	-2740
8	0	0	1929	1904
6	0	0	1096	-1096
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3	1	15	469	-403
-1	1	14	529	541
-3	1	14	642	-598
-13	1	13	400	434
-9	1	13	598	608
-7	1	13	919	-877
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3	1	13	801	762
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7	1	13	1150	1120
9	1	13	878	-868
7	1	12	378	-357
5	1	12	606	601
3	1	12	534	-504
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-9	1	11	1621	-1562
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-3	1	11	1100	1060
-1	1	11	1558	-1547
1	1	11	1633	1647
3	1	11	1563	-1553
5	1	11	1026	1057
7	1	11	623	-623
9	1	11	700	692
11	1	11	752	-719
13	1	11	736	711
11	1	10	433	437
5	1	10	375	371
1	1	10	817	-788
-1	1	10	907	910
-3	1	10	485	-493
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-13	1	10	829	880
-15	1	10	510	-519
-17	1	9	891	860
-15	1	9	1293	-1257
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-9	1	9	710	696
-7	1	9	893	-875
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13	1	7	915	-818
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-12	2	13	484	-512
-14	2	12	575	560
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-12	2	11	560	-511
10	2	11	608	606
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8	2	10	787	-733
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12	2	10	895	-884
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-2	2	6	1059	1041
0	2	6	2096	-2101
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6	2	6	1222	1248

8	2	6	521	-589	4	2	1	2139	-2096	-3	3	10	791	765	-9	3	4	1278	-1296
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-14	2	4	941	-822	16	2	0	1156	-1220	7	3	7	457	-497	15	3	3	870	-873
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4	2	4	596	-641	5	3	14	392	336	-9	3	7	964	-930	3	3	3	2638	-2593
6	2	4	1203	1196	5	3	13	597	542	-13	3	7	531	534	1	3	3	1284	1274
14	2	4	443	433	3	3	13	1108	-1084	-15	3	7	671	-607	-1	3	3	316	262
16	2	4	635	-645	1	3	13	1415	1303	-9	3	6	407	435	-3	3	3	604	632
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18	2	3	456	-499	-3	3	13	239	402	-5	3	6	817	814	-7	3	3	3134	3116
10	2	3	960	-903	-7	3	13	257	343	-3	3	6	908	-849	-9	3	3	2186	-2124
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6	2	3	1625	-1605	-11	3	13	772	674	1	3	6	848	-812	-15	3	3	720	753
2	2	3	770	796	-13	3	12	537	474	3	3	6	1001	988	-17	3	3	1006	-1008
0	2	3	633	-592	-11	3	12	626	-628	5	3	6	1251	-1201	-19	3	3	881	961
-2	2	3	1740	-1785	-9	3	12	861	785	7	3	6	1222	1194	-19	3	2	700	-690
-4	2	3	2389	2431	-7	3	12	858	-876	9	3	6	1113	-1067	-17	3	2	845	841
-6	2	3	1224	-1286	-5	3	12	850	783	11	3	6	776	753	-15	3	2	993	-1020
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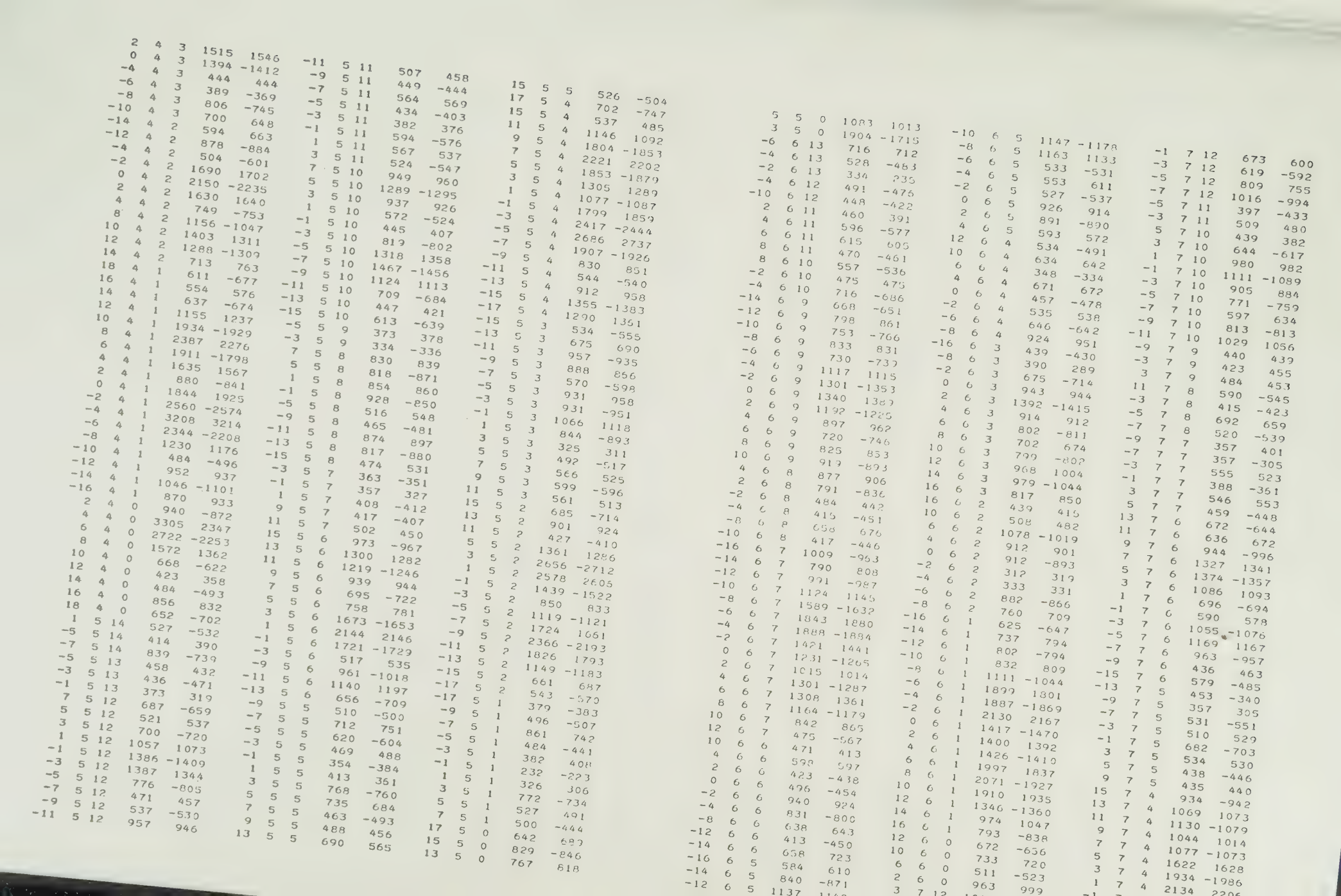

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10	8	7	773	-770	1	9	6	406	355	-2	10	6	1013	-1021
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6	10	2	1134	1108
8	10	2	656	-655
10	10	1	776	772
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6	10	1	783	749
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2	10	1	502	515
0	10	1	514	-607
-2	10	1	769	886
-4	10	1	825	-850
-6	10	1	886	826
-8	10	1	514	-498
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2	10	0	1033	-1073
4	10	0	524	422
10	10	0	705	-715

The Crystal Structure of Dipotassium Tellurate(IV) Trihydrate, $K_2TeO_3 \cdot 3H_2O$.

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(Abstract) $K_2TeO_3 \cdot 3H_2O$ crystallizes in space group Pnma with a = 8.930(3) , b = 6.973(3) , c = 12.481(3) Å , Z = 8. 1336 independent reflexions were used in full matrix least-squares refinement, a final R-value of 0.036 being obtained. The TeO_3^{2-} anion has a pyramidal configuration with Te-O bond distances in the range 1.848-1.852 Å and O-Te-O angles close to 100 °. The potassium atom is surrounded by six oxygen atoms (K-O: 2.684-2.983 Å).

Introduction

A number of tellurate(IV) structures have been studied during recent years and the literature has been reviewed by Johansson (1978). No structural information on tellurous acid, H_2TeO_3, is available. It is possible to precipitate tellurous acid, but the precipitate is unstable and loses water (Dutton & Cooper, 1966). Structures containing free TeO_3^{2-} ions also seem to be rather unstable. The reason for this is that the Te(IV) free $5s^2$ electron pair is probably very easily polarized.

Distortion of the free electron pair leads to rearrangements in the electron density of the pyramidal Te-O bonds in the TeO_3^{2-} ions. The free TeO_3^{2-} ion thus tends to form condensed tellurate(IV) groups, chains, layers or 3-dimensional nets. (Lindqvist & Johansson, 1976).

The Te(IV)-O coordination polyhedra are usually also irregular in the condensed structures and often have one or two extra weak Te-O interactions in addition to three or four strong Te-O bonds (Zeman, 1971).

A detailed understanding of tellurate(IV) chemistry requires knowledge of accurate dimensions for the unpolarized TeO_3^{2-} ion, and we have therefore started structural investigations of ammonium and alkali metal tellurates(IV).

Experimental

The crystals were prepared by melting equimolecular amounts of TeO_2 and K_2CO_3 in a platinum cruicible under CO_2(g). After about 1 hour a crystalline mass was obtained on cooling from which it was possible to separate single crystals of $K_2TeO_3 \cdot 3H_2O$ suitable for an x-ray structure determination. The crystals are very hygroscopic, and dissolve rapidly if the relative humidity exceeds 40 %. If $K_2TeO_3 \cdot 3H_2O$ is allowed to dissolve in humid air, crystals of a new, more stable potassium tellurate(IV) are formed.

It was, however, possible by working in dry air to mount a crystal of $K_2TeO_3 \cdot 3H_2O$ in a glass capillary. Cell dimensions and intensity data were obtained from measurement on a Syntex $P2_1$ diffractometer. Crystallographic and experimental data are listed in Table 1.

The reflections were measured in 96 steps and the intensities were evaluated from a profile analysis according to the Lehmann-Larsen (1974) method using the program LELA (Lindqvist and Ljungström, 1978). The intensities were corrected for Lorentz and polarization effects with a local program (SYN) and the absorption correction was carried out with the program DATAPH (Coppens, Leiserowitz and Rabinovich 1965, modified by Hamilton 1971).

Determination of the structure

The intensity data had systematic extinctions for 0$k$$l$: $k+l = 2n + 1$ and hk0: $h = 2n + 1$, indicating the space group to be either $Pn2_1a$ or $Pnma$. Patterson and electron density calculations showed that the structure belonged to $Pnma$ with all the tellurium and potassium atoms and 1/3 of the oxygen atoms occupying special positions on the mirror planes at $y = 1/4$ and $y = 3/4$ (cf Table 2).

Initially refinement was carried out with the program BLOCK (Lindgren, 1977), and an R value of 0.056 was obtained for a structure model with isotropic temperature factors. The final cycles of refinement were performed with the full matrix least squares program LINUS (Coppens and Hamilton, 1970), including anisotropic temperature factors and an isotropic extinction parameter. The final R value was 0.036 and the corresponding parameters are listed in Table 2*. The scattering factors for Te (Cromer and Waber, 1965), K and O (Doyle and Turner, 1968) were corrected for the real part of the anomalous scattering (Cromer, 1965). The observations were weighted according to the formula:
$w = (20.0 + F_o + 0.004\ F_o^2)^{-1}$ (Cruickshank, 1970), and the corresponding weight analysis is shown in Table 3.

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*Observed and calculated structure factors have been deposited .....

Discussion

$K_2TeO_3 \cdot 3H_2O$ is a purely ionic compound built up from K^+ and TeO_3^{2-} ions and H_2O molecules. The potassium - oxygen interactions are shown in Table 4, and both K(1) and K(2) are seen to have distorted octahedral coordination. The dimensions of the TeO_3^{2-} - ion are compared with those of SO_3^{2-} and SeO_3^{2-} in Table 5.

K(1) only coordinates water oxygen atoms, while K(2) interacts both with water molecules and with two TeO_3^{2-} ions (see Fig 1). The mean K-O coordination distances are 2.806 Å and 2.837 Å for K(1) and K(2) respectively, which is in good agreement with the values 2.72 - 2.91(8) Å given in the International Tables (1962) for six-fold coordination.

In addition to electrostatic forces, the structure is held together by rather strong hydrogen bonds (cf Fig 1 and Table 6).

The TeO_3^{2-} ion in $K_2TeO_3 \cdot 3H_2O$ is pyramidal. Previously, isolated TeO_3^{2-} ions have only been found in $BaTeO_3 \cdot H_2O$ (Rottensten-Nielsen, Grønbaek Hazell and Rasmussen, 1971) and in $Cu(NH_3)TeO_3 \cdot H_2O$ (Johansson and Lindqvist, 1977), and the dimensions are compared in Table 5.

The mean values found in $K_2TeO_3 \cdot 3H_2O$ for the Te-O bond and the O-Te-O angles, 1.851(4) Å and 99.3(2)°, respectively: are to be considered representative for an unpolarized TeO_3^{2-} ion. This statement is supported by the fact that there is no "back-bonding", i.e. interactions between oxygen atoms and the Te(IV) free electron pair, in $K_2TeO_3 \cdot 3H_2O$. The free space on the rear-side of Te(IV) is astonishingly large with no contact shorter than 3.87 Å. In the case of both $BaTeO_3 \cdot H_2O$ and $Cu(NH_3)TeO_3 \cdot H_2O$ weak "backbonding" with Te-O distances of about 3 Å may be considered to occur.

The unsymmetrical octahedral oxygen coordination in $Cu(NH_3)TeO_3 \cdot H_2O$ with three strong interactions on one side and three very weak on the other side of the Te(IV) atom, has also been compared with similar geometries in Te(IV) halogen compounds (Johansson & Lindqvist, 1976). The Te(IV)-O distances of about 3 Å correspond undoubtedly to weak interatomic interactions (Lindqvist & Moret, 1973; Brown, 1974).

The present results for $K_2TeO_3 \cdot 3H_2O$ provide new information concerning the action range of the Te(IV) $5s^2$ free electron pair. Galy, Meunier, Andersson & Åström (1975) have demonstrated that in condensed tellurates(IV) the Te(IV) free electron pair has, on the average, a volume corresponding to that of an oxygen atom. However, condensed tellurates(IV) always exhibit interactions between the Te(IV) free electron pair and neighbouring oxygen atoms; and the spatial distribution of the free electron pair density is probably not spherical. In $K_2TeO_3 \cdot 3H_2O$, on the other hand, there is enough space for a spherical distribution corresponding to a radius of $\sim$ 1.25 Å (assuming a van der Waals' radius for O of 1.4 Å; Pauling 1952). This radius for the free $5s^2$ electron pair (cf. Fig 2) may be used in an approximation of the unpolarized TeO_3^{2-} ion.

We wish to thank Dr Susan Jagner for revising the English text. Financial aid has been provided by the Swedish Natural Science Research Council (NFR).

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Table 1. Experimental data

1. Physical and crystallographic data

Formula:	$K_2TeO_3 \cdot 3H_2O$	a	= 8.930(3)Å
Molecular weight:	307.86	b	= 6.973(3)Å
Space group:	Pnma	c	= 12.481(3)Å
Absorption coefficient	25.12 cm^{-1}	V	= 777.2(4)$Å^3$
Density (calc):	2.515 g cm^{-3}	Z	= 8
Crystals: Hygroscopic, colourless parallelepipeds		F(000)	= 196

2. Data collection

Crystal dimensions:	0.10 x 0.10 x 0.30 mm^3
Radiation:	MoK_α = 0.71069 Å
Monochromator:	Graphite crystal
Scan mode:	w/2θ
Maximum 2θ angle:	60.0 °
Scan interval (Δw):	1.0 ° - 1.2 °
Scan speed (in w):	1.0 °/min - 6.0 °/min
Standard reflection:	(0, 1, 1) in intervals of 25 10500 ± 200 counts, stable
Recorded reflections:	2290
Independent reflections:	1336
Significant reflections:	832 $(I/\sigma(I) > 3.0)$
Cell refinement :	15 reflections with $5.6 < 2\theta < 26.3$ °.

Table 2. Final atomic parameters in $K_2TeO_3 \cdot 3H_2O$

The anisotropic temperature factor is exp $[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2hka^*b^*U_{12} + 2hla^*c^*U_{13} + 2klb^*c^*U_{23})]$
Estimated standard deviations in parantheses. W denotes the oxygen atom in a water molecule.

	$\underline{x}$	$\underline{y}$	$\underline{z}$	$\underline{U}_{11}$	$\underline{U}_{22}$	$\underline{U}_{33}$	$\underline{U}_{12}$	$\underline{U}_{13}$	$\underline{U}_{23}$
Te	-0.00566(7)	1/4	0.21899(5)	0.0226(3)	0.0178(3)	0.0158(3)	-	0.0008(2)	-
K(1)	0.4893(2)	1/4	-0.0974(2)	0.0155(8)	0.0229(9)	0.0280(10)	-	0.0000(8)	-
K(2)	0.0519(2)	1/4	-0.0728(2)	0.01732(8)	0.0231(9)	0.0183(9)	-	0.0008(7)	-
O(1)	0.3564(9)	1/4	0.3926(7)	0.027(4)	0.057(6)	0.029(4)	-	0.008(3)	-
O(2)	0.1081(6)	0.0427(8)	0.1731(5)	0.033(3)	0.018(3)	0.052(4)	0.007(2)	0.001(2)	-0.007(3)
W(1)	0.3033(6)	0.0067(9)	0.0046(4)	0.025(2)	0.028(3)	0.037(3)	0.005(2)	0.003(2)	0.009(2)
W(2)	0.2702(9)	3/4	0.2501(7)	0.032(4)	0.031(4)	0.029(3)	-	-0.001(3)	-

Table 3. Weight analysis after the last cycle of refinement

N is the number of reflexions in the Fo-interval and $w\Delta^2$ are normalized sums.

Fo - interval	N	$w\Delta^2$
0.0 - 15.4	92	2.78
15.4 - 19.7	88	1.90
19.7 - 24.9	82	1.02
24.9 - 29.6	82	1.06
29.6 - 35.8	83	0.39
35.8 - 44.4	83	0.40
44.4 - 54.2	85	0.39
54.2 - 66.1	79	0.33
66.1 - 88.3	77	0.43
88.3 - 297.4	81	1.00

Table 4. Distances (Å) and angles (°) within the potassium coordination polyhedra and oxygen-oxygen contacts. (W denotes the oxygen atom in a water molecule).

K(1) - W(1) x 2	2.684(6)
K(1) - W(1) x 2	2.814(6)
K(1) - W(2)	2.856(8)
K(1) - W(2)	2.983(8)
K(2) - W(2)	2.705(8)
K(2) - O(2) x 2	2.779(6)
K(2) - O(1)	2.830(9)
K(2) - W(1) x 2	2.965(6)

W(1) - K(1) - W(1)	127.8(1) x 2
W(1) - K(1) - W(1)	79.1(2) x 2
W(1) - K(1) - W(1)	78.3(3)
W(1) - K(1) - W(2)	140.7(1) x 2
W(1) - K(1) - W(2)	79.7(2) x 2
W(1) - K(1) - W(1)	78.9(2)
W(1) - K(1) - W(2)	77.2(2) x 2
W(1) - K(1) - W(2)	140.0(1)
W(1) - K(1) - W(2)	140.7(1)
W(2) - K(1) - W(2)	99.2(1)
O(1) - K(2) - O(2)	92.2(2) x 2
O(1) - K(1) - W(1)	102.0(2) x 2
O(1) - K(2) - W(2)	177.9(3)
O(2) - K(2) - O(2)	94.4(3)
O(2) - K(2) - W(1)	161.8(2) x 2
O(2) - K(2) - W(1)	96.4(2) x 2
O(2) - k(2) - W(2)	86.4(2) x 2
W(1) - K(2) - W(1)	69.7(2)
W(1) - K(2) - W(2)	79.7(2) x 2

Table 5. Distances (Å) and angles (°) for Te - O in $BaTeO_3 \cdot H_2O$, $Cu(NH_3)TeO_3 \cdot H_2O$ and $K_2TeO_3 \cdot 3H_2O$

$Cu(NH_3)TeO_3 \cdot H_2O$ [a]		$BaTeO_3 \cdot H_2O$ [b]		$K_2TeO_3 \cdot 3H_2O$	
bond distances					
Te - O(2)	1.870(7)	Te - O(1)	1.858(6)	Te - O(1)	1.848(8)
Te - O(3)	1.877(7)	Te - O(2)	1.847(7)	Te - O(2)	1.852(6) x 2
Te - O(1)	1.885(8)	Te - O(3)	1.859(6)	Te - O(1)	3.872(8)
Te - O(3')	2.950(7)	Te - O(4)	3.035(7)	Te - O(2)	3.959(6) x 2
Te - O(3")	3.082(7)	Te - O(5)	3.332(9)		
Te - O(1')	3.236(9)				
angles					
O(1)-Te-O(2)	96.1(4)	O(1)-Te-O(2)	98.8(3)	O(1)-Te-O(2)	97.7(3)
O(1)-Te-O(3)	94.7(3)	O(1)-Te-O(3)	96.5(3)	O(1)-Te-O(2)	97.7(3)
O(2)-Te-O(3)	97.6(3)	O(2)-Te-O(3)	102.7(3)	O(2)-Te-O(2)	102.4(4)

Distances (Å) and angles (°) for S - O and Se - O in Na_2SO_3 and $CuSeO_3 \cdot 2H_2O$

Na_2SO_3 [c]		$CuSeO_3 \cdot 2H_2O$ [d]	
bond distances			
S - O	1.504(3) x 3	Se - O(1)	1.77(5)
		Se - O(2)	1.78(5)
		Se - O(3)	1.72(5)
angles			
O - S - O	105.69(17)	O(1) - Se - O(2)	98.5
		O(1) - Se - O(3)	103.5
		O(2) - Se - O(3)	96.0

a) Johansson & Lindqvist, (1977)
b) Rottensten-Nielsen, Grønbaek Hazell & Rasmussen (1971)
c) Larsson & Kierkegaard (1969)
d) Gattow (1958)

Table 6. Hydrogen bonding in $K_2TeO_3 \cdot 3H_2O$

O(1) - W(1)	2.671(8) Å x 2
O(2) - W(1)	2.726(8) Å
O(1) - W(1) - O(2)	96.9(3)°
O(2) - W(2)	2.673(8) Å
O(2) - W(1) - O(2)	99.4(4)°

Observed and calculated structure factors for $K_2TeO_3.3H_2O$

0	0	1	48	0	
0	0	2	1077	-1105	
0	0	3	62	0	U
0	0	4	1014	946	
0	0	5	41	0	U
0	0	6	1046	-1029	
0	0	7	68	0	U
0	0	8	76	24	U
0	0	9	71	0	U
0	0	10	701	705	
0	0	11	110	0	U
0	0	12	93	-112	U
0	0	13	67	0	U
0	0	14	625	647	
0	0	15	58	0	U
0	0	16	518	-499	
0	0	17	70	0	U
1	0	0	31	0	U
1	0	1	602	568	
1	0	2	124	136	
1	0	3	1364	-1330	
1	0	4	454	439	
1	0	5	1366	1393	
1	0	6	153	-114	
1	0	7	1501	-1547	
1	0	8	290	-321	
1	0	9	580	601	
1	0	10	60	3	U
1	0	11	829	-841	
1	0	12	39	-71	U
1	0	13	562	580	
1	0	14	95	-15	U
1	0	15	60	77	U
1	0	16	60	18	U
1	0	17	99	-7	U
2	0	0	2221	2345	
2	0	1	48	27	U
2	0	2	1412	-1339	
2	0	3	422	399	
2	0	4	73	107	U
2	0	5	574	554	
2	0	6	1200	-1212	
2	0	7	325	-324	
2	0	8	463	-480	
2	0	9	159	-66	
2	0	10	537	515	
2	0	11	87	-5	U
2	0	12	456	-433	
2	0	13	121	-102	
2	0	14	628	634	
2	0	15	39	99	U
2	0	16	623	-616	
2	0	17	121	63	U
3	0	0	41	0	U
3	0	1	294	275	
3	0	2	327	316	
3	0	3	38	-61	U
3	0	4	700	670	
3	0	5	1706	1688	
3	0	6	117	141	
3	0	7	1024	-1061	
3	0	8	402	-425	
3	0	9	801	806	
3	0	10	67	-23	U
3	0	11	791	-808	
3	0	12	146	-140	
3	0	13	607	599	
3	0	14	68	57	U
3	0	15	136	140	U
3	0	16	145	122	
4	0	0	1915	1795	
4	0	1	54	51	U
4	0	2	992	-993	
4	0	3	169	150	
4	0	4	1045	990	
4	0	5	372	363	
4	0	6	1012	-991	
4	0	7	86	18	U
4	0	8	161	154	
4	0	9	280	-261	
4	0	10	433	438	
4	0	11	169	-174	
4	0	12	352	-347	
4	0	13	263	-249	
4	0	14	546	530	
4	0	15	172	161	
4	0	16	539	-504	
5	0	0	63	0	U
5	0	1	567	-545	
5	0	2	465	458	
5	0	3	632	-581	
5	0	4	189	187	
5	0	5	934	930	
5	0	6	312	346	
5	0	7	1006	-1000	
5	0	8	304	-297	
5	0	9	639	628	
5	0	10	131	-153	
5	0	11	925	-898	
5	0	12	162	-193	
5	0	13	288	282	
5	0	14	120	92	U
5	0	15	60	-19	U
5	0	16	88	130	U
6	0	0	1254	1257	
6	0	1	459	473	
6	0	2	724	-712	
6	0	3	155	-156	
6	0	4	497	516	
6	0	5	313	308	
6	0	6	466	-461	
6	0	7	160	169	
6	0	8	208	208	
6	0	9	107	-110	
6	0	10	524	530	
6	0	11	178	-180	
6	0	12	416	-415	
6	0	13	144	-157	
6	0	14	361	342	
6	0	15	172	148	
7	0	0	37	0	U
7	0	1	76	-22	U
7	0	2	518	519	
7	0	3	366	-378	
7	0	4	71	-18	U
7	0	5	1086	1061	
7	0	6	201	204	
7	0	7	389	-402	
7	0	8	320	-315	
7	0	9	719	694	
7	0	10	37	-90	U
7	0	11	538	-569	
7	0	12	108	-119	U
7	0	13	209	196	
7	0	14	67	71	U
8	0	0	835	812	
8	0	1	267	263	
8	0	2	953	-951	
8	0	3	45	-96	U
8	0	4	289	275	
8	0	5	84	74	U
8	0	6	343	-333	
8	0	7	130	114	
8	0	8	115	115	U
8	0	9	34	-105	U
8	0	10	279	288	
8	0	11	56	4	U
8	0	12	347	-351	
8	0	13	176	-183	
9	0	0	85	0	U
9	0	1	223	-212	
9	0	2	308	311	
9	0	3	402	-426	
9	0	4	35	-4	U
9	0	5	823	831	
9	0	6	125	122	
9	0	7	278	-279	
9	0	8	293	-283	
9	0	9	403	404	
9	0	10	140	110	
9	0	11	469	-469	
9	0	12	17	-10	U
10	0	0	585	600	
10	0	1	105	122	U
10	0	2	502	-497	
10	0	3	310	-317	
10	0	4	361	372	
10	0	5	135	118	
10	0	6	57	-4	U
10	0	7	58	1	U
10	0	8	189	167	
10	0	9	107	55	U
10	0	10	281	279	
11	0	0	42	0	U
11	0	1	200	-213	
11	0	2	89	64	U
11	0	3	266	-271	
11	0	4	85	-82	U
11	0	5	517	545	
11	0	6	45	71	U
11	0	7	190	-205	
11	0	8	221	-222	
12	0	0	294	303	
12	0	1	28	-27	U
12	0	2	375	-384	
12	0	3	334	-323	
12	0	4	168	160	
12	0	5	27	20	U
0	1	0	49	0	U
0	1	1	1200	-1218	
0	1	2	65	0	U
0	1	3	2073	2170	
0	1	4	42	0	U
0	1	5	96	-135	U
0	1	6	49	0	U
0	1	7	200	-172	
0	1	8	43	0	U
0	1	9	258	-149	
0	1	10	64	0	U
0	1	11	742	-751	
0	1	12	42	0	U
0	1	13	717	701	
0	1	14	71	0	U
0	1	15	490	-467	
0	1	16	7	0	U
0	1	17	575	569	
1	1	0	66	0	U
1	1	1	118	-112	
1	1	2	1073	-1054	
1	1	3	75	-84	U
1	1	4	1282	1314	
1	1	5	89	-11	U
1	1	6	840	-836	
1	1	7	87	73	U
1	1	8	1341	1374	
1	1	9	174	170	
1	1	10	1128	-1131	
1	1	11	115	-59	
1	1	12	240	224	
1	1	13	68	-81	U
1	1	14	348	-358	
1	1	15	24	-53	U
1	1	16	186	198	
1	1	17	78	1	U
2	1	0	127	-106	
2	1	1	1466	-1378	
2	1	2	117	-111	
2	1	3	2571	2571	
2	1	4	66	-71	U
2	1	5	651	-648	
2	1	6	40	41	U
2	1	7	30	6	U
2	1	8	244	253	
2	1	9	259	-280	
2	1	10	176	175	
2	1	11	468	-480	
2	1	12	155	-167	
2	1	13	632	650	
2	1	14	111	-97	U
2	1	15	438	-429	
2	1	16	144	-107	
2	1	17	440	459	
3	1	0	63	0	U
3	1	1	452	-421	
3	1	2	611	-614	
3	1	3	85	-80	U
3	1	4	974	971	
3	1	5	329	344	
3	1	6	975	-968	
3	1	7	175	181	
3	1	8	1215	1215	
3	1	9	236	263	
3	1	10	920	-928	
3	1	11	168	-167	
3	1	12	336	334	
3	1	13	114	-127	
3	1	14	326	-340	
3	1	15	95	-97	U
3	1	16	35	88	U
4	1	0	177	-170	
4	1	1	752	-734	
4	1	2	498	-497	
4	1	3	1636	1605	
4	1	4	265	273	
4	1	5	528	-532	
4	1	6	120	124	
4	1	7	186	-183	
4	1	8	248	267	
4	1	9	83	-23	U
4	1	10	99	89	U
4	1	11	413	-403	
4	1	12	162	-167	
4	1	13	729	706	
4	1	14	96	-106	U
4	1	15	536	-495	
4	1	16	122	-148	U
5	1	0	57	0	U
5	1	1	537	-524	
5	1	2	762	-744	
5	1	3	127	-131	
5	1	4	534	533	
5	1	5	597	601	
5	1	6	790	-794	
5	1	7	166	158	
5	1	8	1157	1139	
5	1	9	163	157	
5	1	10	642	-673	
5	1	11	210	-233	
5	1	12	348	347	
5	1	13	115	-84	U
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4	7	8	94	-123	U
4	7	9	92	-17	U
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2	8	8	143	-125	
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3	8	0	61	0	U
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3	8	2	188	194	
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3	8	5	578	589	
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6	8	5	170	170	
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0	9	7	101	-79	U
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2	9	4	27	33	U
2	9	5	207	-175	
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3	9	0	116	0	U
3	9	1	68	-104	U
3	9	2	217	-216	
3	9	3	93	14	U
3	9	4	283	280	
3	9	5	127	102	U
4	9	0	36	-56	U
4	9	1	309	-286	
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4	9	3	490	467	
4	9	4	101	52	U
5	9	0	122	0	U

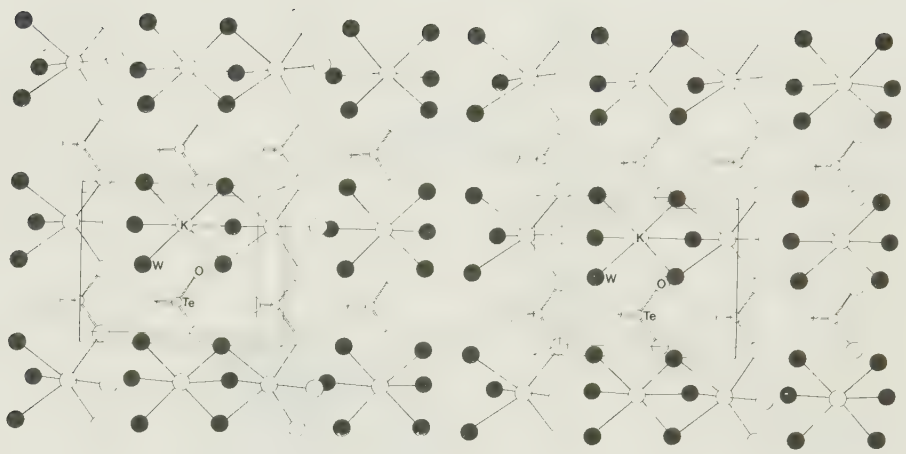

Fig. 1.

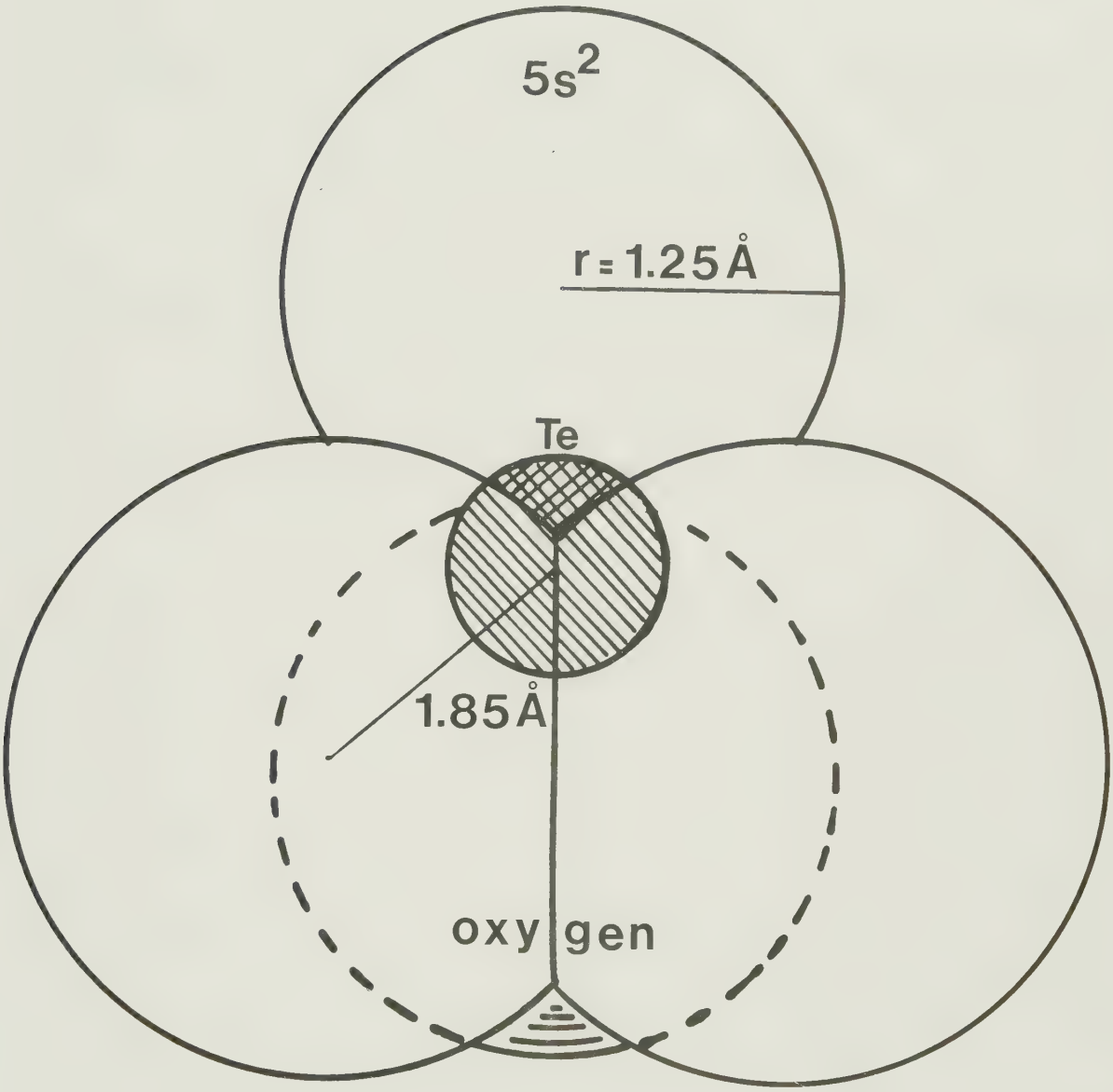

Fig. 2.

Figure legends.

Figure 1. A stereoscopic picture of the structure projected along the c axis (ORTEP; Johnson, 1965). W denotes the oxygen atom in a water molecule.

Figure 2. The TeO_3^{2-} ion indicating the estimated radius of the $5s^2$ free electron pair.

Diammonium Ditellurium(IV) Pentaoxide Dihydrate

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Abstract

$(NH_4)_2Te_2O_5 \cdot 2H_2O$, monoclinic, $P2_1/c$, a = 10.357(3), b = 11.000(3), c = 8.178(2) Å, β = 93.23(1)°, Z = 4, V = 930.2(2) Å^3, D_x = 2.91 g cm^{-3} and M_r = 407.30. Least-squares refinement based on 2439 independent reflections gave R = 0.031. The Te_2O_5 groups are connected to form chains, the Te – O bond distances within the Te_2O_5 group ranging from 1.834(4) to 2.034(3) Å, while the Te – O bridging distances are 2.218(3) and 2.506(4) Å. The coordination of the two independent Te(IV) atoms is four-fold and can be described as distorted trigonal bipyramidal with the free $5s^2$ electron pair occupying one of the equatorial positions.

Introduction

The preparation of crystalline ammonium tellurate(IV) was described by Lehner & Wolesensky (1913) who suggested the formula $(NH_4)_2TeO_3$. In the present investigation, single crystals of composition $(NH_4)_2Te_2O_5 \cdot 2H_2O$ were prepared by hydrothermal synthesis. TeO_2(s) was mixed with an excess of concentrated ammonia and held in an autoclave at 100 °C for 24 h., colourless, prismatic crystals,

suitable for X-ray work, being obtained. The crystals are unstable in air and were therefore mounted in glass capillaries in a glove-box containing $NH_3(g)$. If the autoclave is opened in air, the $(NH_4)_2Te_2O_5 \cdot 2H_2O$ crystals deliquesce, a new phase, hexagonal $(NH_4)_2Te_4O_9 \cdot 4H_2O$, being subsequently formed. These crystals are stable in air and their crystal structure is under investigation.

A single crystal of dimensions 0.10 x 0.09 x 0.19 mm^3 was used for data collection with a Syntex $P2_1$ diffractometer (cf. Table 1). The integrated intensities were evaluated according to the Lehmann-Larsen (1974) profile analysis method using a local program, LELA (Lindqvist & Ljungström, 1978). The intensities were corrected for Lp effects with a local program (SYN), but it was not possible to apply a correction for absorption as the crystal was submerged in epoxy-glue within the glass capillary.

The structure was solved from Patterson and electron density calculations (program DRF; A. Zalkin, Berkeley). The systematic absences $\underline{l} = 2\underline{n} + 1$ for $\underline{h}0\underline{l}$ and $\underline{k} = 2\underline{n} + 1$ for $0\underline{k}0$ indicated that the space group was $\underline{P}2_1/\underline{c}$. The structural parameters were refined with a block-diagonal approximation program (BLOCK; Lindgren, 1977). Refinement with isotropic temperature factors gave $\underline{R} = 0.060$ and when anisotropic temperature factors were included $\underline{R}$ dropped to 0.036. This relatively large difference and the low $\underline{B}$ values for Te (cf. Table 2) indicate that the anisotropic temperature factors may be influenced by absorption effects. It was evident that a few strong reflections were subject to secondary extinction. Eight such reflections were therefore discarded giving a final $\underline{R}$ of 0.031. The corresponding structural parameters are listed in Table 2.*

*A list of observed and calculated structure factors has been deposited.

Atomic scattering factors due to Cromer & Waber (1965) were used for Te, while the values given by Doyle & Turner (1968) were used for O and N. The real part of the anomalous scattering for Te (Cromer, 1965) was taken into account. Weights were calculated according to the formula $\underline{w} = (\underline{a} + \underline{F}_o + \underline{c}\underline{F}_o^2 + \underline{d}\underline{F}_o^3)^{-1}$ (Cruickshank, 1970) with $\underline{a}$ = 40.0, $\underline{b}$ = 0.04 and $\underline{d}$ = 0.0001. The corresponding weight analysis is given in Table 3.

Discussion

Interatomic distances and angles were calculated with the program DISTAN (A. Zalkin, Berkeley) and are presented in Fig. 1 and Table 4. The structure of $(NH_4)_2Te_2O_5 \cdot 2H_2O$ consists of Te_2O_5 groups connected *via* double oxygen bridges to form chains (cf. Fig. 2). The chains are held together by hydrogen bonds involving the ammonium ions and the water molecules (cf. Fig. 3).

The coordination of the two independent tellurium atoms in the structure can be described as four-fold. The four tellurium - oxygen bonds are directed towards the axial and two of the equatorial corners of a trigonal bipyramid. The third corner in the equatorial plane is occupied by the $5s^2$ free electron pair. According to Lindqvist (1968) the axial bonds are significantly longer than the equatorial bonds, which are 2.10 Å and 1.90 Å, respectively, in α-TeO_2. The coordination around Te(1) is a good example of Te(IV) four-fold coordination (cf. Fig. 1) while that of Te(2) has elements of three-fold coordination, one of the axial bonds being short (Te(2) - O(7) = 1.971(4) Å) and the other being considerably longer (Te(2) - O"(9) = 2.506(4) Å).

The ideal O_{ax} - Te - O_{ax} and O_{eq} - Te - O_{eq} angles are 180° and 120°, respectively, but the repulsion between the bonding electrons and the free electron pair results in decreased angles. In $(NH_4)_2Te_2O_5 \cdot 2H_2O$ the axial and equatorial angles (cf. Table 4) compare well with the values found in α-TeO_2 (Lindqvist, 1968) and in β-TeO_2 (Beyer, 1967) in which they are 101 - 102° (eq) and 168 - 169° (ax).

Another comparable structure with four-fold Te(IV) coordination is $Te_2O_4 \cdot HNO_3$ (Swink & Carpenter, 1966), in which Te_2O_4 groups are connected via double oxygen bridges to form layers. The angle around the oxygen atom with strong bonds to both tellurium atoms within the group is 126.2(8)° (2x) in $Te_2O_4 \cdot HNO_3$ which is to be compared with 118.1(2)° for Te(1) - O(7) - Te(2) in $(NH_4)_2Te_2O_5 \cdot 2H_2O$. The corresponding angle in $Te_2O_3SO_4$ (Johansson & Lindqvist, 1976) is 134.9(7)°. In $Te_2O_3SO_4$ Te_2O_5 units are also connected to form chains, but the oxygen coordination around tellurium is different.

The hydrogen bonds within the structure are probably as indicated in Table 5 in which relevant O - O and N - O distances are given. A neutron diffraction study of $(NH_4)_2Te_2O_5 \cdot 2H_2O$ is in progress to elucidate the detailed structure of the water molecules and the ammonium ions.

The author wishes to thank Prof. Oliver Lindqvist and Dr Jacques Moret for valuable discussions and Dr Susan Jagner for revising the English text. Financial support has been obtained from the Swedish Natural Science Research Council (NFR, Contract No 3396).

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Table 1. Crystallographic and experimental data.

1. Physical and crystallographic data

Formula:	$(NH_4)_2Te_2O_5 \cdot 2H_2O$	a =	10.357(3) Å
Molecular weight:	407.22	b =	11.000(3) Å
Space group:	$P2_1/c$	c =	8.178(2) Å
Density (calc.):	2.91 g cm^{-3}	β =	93.23(1)°
Crystal morphology:	Colourless prisms	V =	930.2(2) $Å^3$
		Z =	4

2. Data collection

Crystal dimensions:	0.10 x 0.09 x 0.19 mm^3
Radiation:	MoK_α = 0.71069 Å
Monochromator:	Graphite crystal
Scan mode:	w/2θ
Maximum 2θ angle:	60.0°
Scan interval (Δw):	2.4 - 3.6°
Scan speed (in w):	2.0°/min - 12.0°/min
Standard reflection:	(1,1,3) at intervals of 25 reflection
	67000 ± 1500 counts, stable
Recorded reflections:	3040
Independent reflections:	2828
Significant reflections:	2439 (I/σ (I)) > 3.0)
Refinement of cell parameters:	15 reflections with 12.4° < 2θ < 27.4

Table 2. Final atomic parameters in $(NH_4)_2Te_2O_5 \cdot 2H_2O$. The anisotropic factor is $\exp[-2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}l^2c^{*2} + U_{12}hka^*b^* + U_{13}hla^*c^* + U_{23}hlb^*c^*)] \cdot 10^4$. Estimated standard deviations are given in parentheses (W(1) and W(2) denote the oxygen atoms in the two water molecules).

Atom	x/a	y/b	z/c
Te(1)	0.08168(3)	0.07289(2)	0.12346(2)
Te(2)	0.61033(3)	-0.01038(2)	0.64698(2)
W(1)	0.1236(6)	0.3678(4)	0.0822(5)
O(2)	0.7930(4)	0.4370(3)	0.0739(3)
O(3)	0.4991(5)	0.5850(3)	0.0843(3)
N(1)	0.1850(6)	0.7161(4)	0.1610(4)
W(2)	0.2807(7)	0.3103(5)	0.3344(5)
O(6)	0.9232(4)	0.6501(3)	0.3119(3)
O(7)	0.6538(4)	0.4907(3)	0.3021(3)
N(2)	0.4553(6)	0.6438(4)	0.4552(4)
O(9)	0.1634(5)	0.4996(3)	0.4741(3)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Te(1)	177(1)	189(1)	175(1)	-9(2)	-20(2)	27(2)
Te(2)	189(1)	171(1)	153(1)	-44(2)	-4(2)	3(2)
W(1)	374(24)	485(23)	515(22)	199(40)	52(38)	388(41)
O(2)	194(18)	328(17)	257(14)	466(27)	52(26)	-22(25)
O(3)	281(19)	226(13)	215(13)	129(25)	160(25)	-79(22)
N(1)	297(25)	271(18)	305(18)	6(33)	101(33)	-34(31)
W(2)	477(30)-	548(27)	553(25)	325(48)	100(44)	197(40)
O(6)	272(18)	213(13)	261(14)	-20(26)	-1(26)	30(24)
O(7)	202(18)-	324(16)	183(12)	51(26)	-78(24)	116(24)
N(2)	341(25)	270(18)	305(18)	40(35)	113(34)	164(31)
O(9)	243(18)	382(18)	155(19)	-19(28)	-34(25)	0(24)

Table 3. Weight analysis after the last cycle of refinement.

The quantities $w\Delta^2$ are normalized sums for N reflections within each Fo-interval.

Fo-interval	$w\Delta^2$	N
0.1 - 13.4	1.698	232
13.4 - 19.3	0.701	246
19.3 - 25.8	0.496	246
25.8 - 32.8	0.539	246
32.8 - 39.9	0.668	246
39.9 - 49.5	0.741	246
49.5 - 59.7	1.066	246
59.7 - 72.5	0.902	246
72.5 - 99.1	1.070	246
99.1 - 623.7	2.119	239

Table 4. Distances (Å) and angles (°) within the Te - O coordination polyhedra in $(NH_4)_2Te_2O_5 \cdot 2H_2O$ (cf. Fig. 1).

Te(1)	- O(2)	1.834(4)	O(2) - Te(1) - O(3')	88.0(1)
	- O(3)	1.899(3)	O(2) - Te(1) - O(3)	102.4(2)
	- O(7)	2.034(3)	O(2) - Te(1) - O(7)	90.3(2)
	- O(3')	2.218(3)	O(3) - Te(1) - O(3')	76.4(1)
	- W(1)	3.292(5)	O(3')- Te(1) - O(7)	163.3(1)
			O(3) - Te(1) - O(7)	87.8(1)
Te(2)	- O(6)	1.840(3)		
	- O(9)	1.870(3)	O(6) - Te(2) - O(7)	95.1(2)
	- O(7)	1.971(4)	O(6) - Te(2) - O(9')	86.2(1)
	- O(9')	2.506(4)	O(6) - Te(2) - O(9)	101.9(2)
	O(2)	3.010(4)	O(7) - Te(2) - O(9')	165.2(1)
	W(1)	3.420(5)	O(7) - Te(2) - O(9)	88.8(2)
			O(9) - Te(2) - O(9')	76.5(2)

Table 5. Possible hydrogen bonds. (W(1) and W(2) denote the oxygen atoms in the two water molecules.

W(1) - O(2)	2.796(6) Å	O(2) - W(1) - O(2)	92.3(2) °
- O(2)	2.805(6)	O(2) - W(1) - W(2)	117.5(2)
- W(2)	2.914(7)	O(2) - W(1) - W(2)	125.1(2)
W(2) - O(9)	2.740(6)	W(1) - W(2) - N(2)	150.6(2)
- W(1)	2.914(7)	W(1) - W(2) - N(2)	116.1(2)
- N(2)	3.022(7)	N(2) - W(2) - O(9)	75.5(2)
N(1) - O(3)	2.756(6)	O(2) - N(1) - O(3)	55.6(1)
- O(6)	2.817(6)	O(2) - N(1) - O(3)	105.8(2)
- O(6)	2.838(6)	O(2) - N(1) - O(6)	113.0(2)
- O(2)	2.973(6)	O(2) - N(1) - O(6)	132.2(2)
- O(3)	3.089(6)	O(3) - N(1) - O(3)	138.6(2)
		O(3) - N(1) - O(6)	133.8(2)
N(2) - O(6)	2.714(5)	O(3) - N(1) - O(6)	80.2(2)
- O(7)	2.877(6)	O(3) - N(1) - O(6)	86.6(2)
- O(9)	2.883(6)	O(3) - N(1) - O(6)	95.6(2)
- W(2)	3.022(7)	O(6) - N(1) - O(6)	110.3(2)
- O(7)	3.092(6)		
		W(2) - N(2) - O(6)	107.3(2)
		W(2) - N(2) - O(7)	95.3(2)
		W(2) - N(2) - O(7)	73.8(2)
		W(2) - N(2) - O(9)	127.1(2)
		O(6) - N(2) - O(7)	103.2(2)
		O(6) - N(2) - O(7)	145.2(2)
		O(6) - N(2) - O(9)	116.2(2)
		O(7) - N(2) - O(7)	111.5(2)
		O(7) - N(2) - O(9)	102.2(2)
		O(7) - N(2) - O(9)	53.3(1)

Observed and calculated structure factors for $(NH_4)_2Te_2O_5.2H_2O$.

1 0 0	249 240	3 2 0	910 829	5 4 0	465 423
2 0 0	222 -220	4 2 0	1844-1957	6 4 0	1153 1113
3 0 0	568 590	5 2 0	929 -862	7 4 0	1100-1088
4 0 0	2449-3109 UE	6 2 0	719 668	8 4 0	279 272
5 0 0	1707-1852	7 2 0	797 -791	9 4 0	107 107
6 0 0	900 941	8 2 0	1006 1016	10 4 0	745 -728
7 0 0	554 -567	9 2 0	778 776	11 4 0	562 555
8 0 0	1083 1105	10 2 0	627 -621	12 4 0	142 150
9 0 0	1098 1117	11 2 0	316 306	13 4 0	363 -346
10 0 0	675 -683	12 2 0	360 -352	14 4 0	417 419
11 0 0	155 171	13 2 0	658 -660	-13 5 0	316 -328
12 0 0	484 -497	14 2 0	417 428	-12 5 0	182 188
13 0 0	668 -699	-14 3 0	455 -469	-11 5 0	250 265
14 0 0	376 394	-13 3 0	358 -376	-10 5 0	491 503
-14 1 0	253 -274	-12 3 0	141 147	-9 5 0	554 569
-13 1 0	173 -180	-11 3 0	376 382	-8 5 0	338 -341
-12 1 0	68 95 U	-10 3 0	637 662	-7 5 0	340 -349
-11 1 0	180 189	-9 3 0	688 698	-6 5 0	698 -704
-10 1 0	342 356	-8 3 0	151 -150	-5 5 0	869 -867
-9 1 0	317 305	-7 3 0	758 -772	-4 5 0	348 322
-8 1 0	178 -186	-6 3 0	914 -962	-3 5 0	855 851
-7 1 0	497 -505	-5 3 0	1098-1149	-2 5 0	338 319
-6 1 0	303 -296	-4 3 0	183 173	-1 5 0	1266 1256
-5 1 0	502 -504	-3 3 0	1239 1285	0 5 0	20 0 U
-4 1 0	489 429	-2 3 0	1621 1695	1 5 0	1297-1256
-3 1 0	633 670	-1 3 0	1496 1517	2 5 0	350 -319
-2 1 0	594 657	0 3 0	81 0	3 5 0	910 -851
-1 1 0	487 550	1 3 0	1576-1517	4 5 0	372 -322
0 1 0	133 0	2 3 0	1724-1695	5 5 0	925 867
1 1 0	563 -550	3 3 0	1343-1285	6 5 0	736 704
2 1 0	658 -657	4 3 0	207 -173	7 5 0	375 349
3 1 0	693 -670	5 3 0	1192 1149	8 5 0	349 341
4 1 0	517 -429	6 3 0	992 962	9 5 0	604 -569
5 1 0	530 504	7 3 0	798 772	10 5 0	521 -503
6 1 0	316 296	8 3 0	158 150	11 5 0	260 -265
7 1 0	518 505	9 3 0	711 -698	12 5 0	194 -188
8 1 0	177 186	10 3 0	680 -662	13 5 0	338 328
9 1 0	330 -305	11 3 0	397 -382	-13 6 0	27 -23 U
10 1 0	338 -356	12 3 0	135 -147	-12 6 0	398 408
11 1 0	184 -189	13 3 0	387 376	-11 6 0	679 690
12 1 0	119 -95	14 3 0	455 469	-10 6 0	635 -653
13 1 0	170 180	-14 4 0	390 419	-9 6 0	136 -151
14 1 0	265 274	-13 4 0	342 -346	-8 6 0	463 -470
-14 2 0	404 428	-12 4 0	149 150	-7 6 0	1223-1270
-13 2 0	624 -660	-11 4 0	533 555	-6 6 0	998 1024
-12 2 0	354 -352	-10 4 0	700 -728	-5 6 0	667 679
-11 2 0	299 306	-9 4 0	109 107	-4 6 0	387 371
-10 2 0	597 -621	-8 4 0	253 272	-3 6 0	1913 1999
-9 2 0	743 776	-7 4 0	1033-1088	-2 6 0	518 -478
-8 2 0	969 1016	-6 4 0	1088 1113	-1 6 0	2117-2165
-7 2 0	748 -791	-5 4 0	429 423	0 6 0	357 325
-6 2 0	646 668	-4 4 0	614 -608	1 6 0	2148-2165
-5 2 0	869 -862	-3 4 0	1361 1434	2 6 0	539 -478
-4 2 0	1686-1957 UE	-2 4 0	642 -578	3 6 0	2003 1999
-3 2 0	837 829	-1 4 0	1479-1507	4 6 0	420 371
-2 2 0	98 -79	0 4 0	998 1039	5 6 0	700 679
-1 2 0	347 -328	1 4 0	1535-1507	6 6 0	1057 1024
0 2 0	2463 3358 UE	2 4 0	665 -578	7 6 0	1351-1270
1 2 0	120 -328 U	3 4 0	1461 1434	8 6 0	495 -470
2 2 0	330 -79 U	4 4 0	644 -608	9 6 0	148 -151
10 6 0	682 -653	-7 9 0	394 398	8 11 0	327 321
11 6 0	726 690	-6 9 0	948 962	9 11 0	7 12 U
12 6 0	414 408	-5 9 0	12 21 U	10 11 0	421 422
13 6 0	65 -23 U	-4 9 0	301 286	-9 12 0	350 365
-13 7 0	71 -82 U	-3 9 0	291 -285	-8 12 0	449 459
-12 7 0	225 225	-2 9 0	1095-1066	-7 12 0	169 -153
-11 7 0	213 -220	-1 9 0	145 -143	-6 12 0	263 276
-10 7 0	116 -110	0 9 0	52 0 U	-5 12 0	350 -344
-9 7 0	195 199	1 9 0	146 143	-4 12 0	772 -754
-8 7 0	347 -351	2 9 0	1102 1066	-3 12 0	157 160
-7 7 0	132 128	3 9 0	297 285	-2 12 0	104 -104
-6 7 0	353 354	4 9 0	291 -286	-1 12 0	18 1 U
-5 7 0	398 -391	5 9 0	10 -21 U	0 12 0	1035 1016
-4 7 0	372 377	6 9 0	993 -962	1 12 0	50 1 U
-3 7 0	202 195	7 9 0	410 -398	2 12 0	117 -104
-2 7 0	641 -597	8 9 0	300 292	3 12 0	180 160
-1 7 0	518 486	9 9 0	52 68 U	4 12 0	778 -754
0 7 0	46 0 U	10 9 0	587 547	5 12 0	362 -344
1 7 0	518 -486	11 9 0	481 486	6 12 0	276 276
2 7 0	651 597	-11 10 0	301 300	7 12 0	161 -153
3 7 0	206 -195	-10 10 0	409 -402	8 12 0	467 459
4 7 0	390 -377	-9 10 0	105 99	9 12 0	372 365
5 7 0	414 391	-8 10 0	194 191	-7 13 0	244 252
6 7 0	376 -354	-7 10 0	549 -551	-6 13 0	338 345
7 7 0	132 -128	-6 10 0	480 488	-5 13 0	344 -349
8 7 0	359 351	-5 10 0	145 128	-4 13 0	139 130
9 7 0	225 -199	-4 10 0	442 -440	-3 13 0	53 -43 U
10 7 0	117 110	-3 10 0	642 628	-2 13 0	677 -680
11 7 0	235 220	-2 10 0	224 -219	-1 13 0	256 266
12 7 0	231 -225	-1 10 0	532 -514	0 13 0	17 0 U
13 7 0	56 82 U	0 10 0	633 606	1 13 0	265 -266
-12 8 0	330 342	1 10 0	544 -514	2 13 0	693 680
-11 8 0	589 606	2 10 0	228 -219	3 13 0	64 45 U
-10 8 0	514 -530	3 10 0	660 628	4 13 0	125 -130
-9 8 0	150 -161	4 10 0	462 -440	5 13 0	366 349
-8 8 0	334 -330	5 10 0	140 128	6 13 0	346 -345
-7 8 0	990-1004	6 10 0	514 488	7 13 0	245 -252
-6 8 0	659 654	7 10 0	562 -551	-6 14 0	189 186
-5 8 0	586 573	8 10 0	211 191	-5 14 0	371 -369
-4 8 0	246 243	9 10 0	121 99	-4 14 0	711 -703
-3 8 0	1356 1349	10 10 0	401 -402	-3 14 0	66 -59 U
-2 8 0	260 -245	11 10 0	301 300	-2 14 0	58 -54 U
-1 8 0	1441-1436	-10 11 0	413 -422	-1 14 0	152 148
0 8 0	120 122	-9 11 0	32 -12 U	0 14 0	1003 979
1 8 0	1486-1436	-8 11 0	322 -321	1 14 0	139 148
2 8 0	251 -245	-7 11 0	497 506	2 14 0	63 -54 U
3 8 0	1377 1349	-6 11 0	777 770	3 14 0	58 -59 U
4 8 0	248 243	-5 11 0	55 -50 U	4 14 0	721 -703
5 8 0	621 573	-4 11 0	283 280	5 14 0	382 -369
6 8 0	693 654	-3 11 0	351 -340	6 14 0	193 186
7 8 0	1041-1004	-2 11 0	1311-1277	-3 15 0	249 249
8 8 0	352 -330	-1 11 0	48 -24 U	-2 15 0	163 -155
9 8 0	176 -161	0 11 0	51 0 U	-1 15 0	414 409
10 8 0	541 -530	1 11 0	28 24 U	0 15 0	28 0 U
11 8 0	628 606	2 11 0	1319 1277	1 15 0	409 -409
12 8 0	340 342	3 11 0	351 340	2 15 0	146 155
-11 9 0	476 -486	4 11 0	286 -280	3 15 0	254 -249
-10 9 0	536 -547	5 11 0	53 50 U	-14 0 1	43 0 U
-9 9 0	67 -68 U	6 11 0	777 -770	-13 0 1	33 0 U
-8 9 0	291 -292	7 11 0	507 -506	-12 0 1	35 0 U

-11	0	1	68	0	U
-10	0	1	41	0	U
-9	0	1	41	0	U
-8	0	1	25	0	U
-7	0	1	42	0	U
-6	0	1	10	0	U
-5	0	1	32	0	U
-4	0	1	78	0	U
-3	0	1	47	0	U
-2	0	1	52	0	U
-1	0	1	22	0	U
0	0	1	49	0	U
1	0	1	27	0	U
2	0	1	47	0	U
3	0	1	77	0	U
4	0	1	26	0	U
5	0	1	57	0	U
6	0	1	32	0	U
7	0	1	24	0	U
8	0	1	59	0	U
9	0	1	52	0	U
10	0	1	49	0	U
11	0	1	37	0	U
12	0	1	35	0	U
13	0	1	19	0	U
14	0	1	28	0	U
-14	1	1	633	-642	
-13	1	1	338	-338	
-12	1	1	92	-100	
-11	1	1	787	-804	
-10	1	1	978	982	
-9	1	1	842	842	
-8	1	1	125	-119	
-7	1	1	1204	1234	
-6	1	1	859	-855	
-5	1	1	1998	-2256	
-4	1	1	740	728	
-3	1	1	1247	-1292	
-2	1	1	300	92	U
-1	1	1	2208	3693	UE
0	1	1	98	82	
1	1	1	44	248	U
2	1	1	725	654	
3	1	1	2337	-2810	UE
4	1	1	1239	-1193	
5	1	1	476	390	
6	1	1	927	-911	
7	1	1	1685	1803	
8	1	1	876	883	
9	1	1	336	-331	
10	1	1	423	410	
11	1	1	613	-612	
12	1	1	908	-933	
13	1	1	441	450	
14	1	1	135	-130	
-14	2	1	346	-351	
-13	2	1	27	-11	U
-12	2	1	172	169	
-11	2	1	542	551	
-10	2	1	737	755	
-9	2	1	105	110	
-8	2	1	214	-215	
-7	2	1	672	-703	
-6	2	1	889	-919	
-5	2	1	588	-580	
-4	2	1	580	605	
-3	2	1	695	757	
-2	2	1	719	796	
-1	2	1	192	202	
0	2	1	723	-747	
1	2	1	1238	-1263	
2	2	1	1116	-1076	
3	2	1	591	424	
4	2	1	713	654	
5	2	1	1148	1099	
6	2	1	991	974	
7	2	1	268	263	
8	2	1	641	-640	
9	2	1	591	-562	
10	2	1	596	-600	
11	2	1	357	-370	
12	2	1	293	290	
13	2	1	349	368	
14	2	1	268	283	
-14	3	1	402	-433	
-13	3	1	53	52	U
-12	3	1	297	298	
-11	3	1	820	-848	
-10	3	1	687	703	
-9	3	1	207	206	
-8	3	1	775	-791	
-7	3	1	992	1066	
-6	3	1	235	-239	
-5	3	1	1335	-1448	
-4	3	1	1251	1343	
-3	3	1	325	-358	
-2	3	1	872	-833	
-1	3	1	2251	2690	U
0	3	1	888	-859	
1	3	1	139	-115	
2	3	1	637	658	
3	3	1	1399	-1425	
4	3	1	288	-251	
5	3	1	634	609	
6	3	1	1113	-1087	
7	3	1	945	939	
8	3	1	258	242	
9	3	1	651	-630	
10	3	1	724	714	
11	3	1	216	-210	
12	3	1	520	-522	
13	3	1	540	542	
14	3	1	230	-248	
-14	4	1	421	-414	
-13	4	1	55	8	U
-12	4	1	174	185	
-11	4	1	655	667	
-10	4	1	715	722	
-9	4	1	47	-9	U
-8	4	1	238	-243	
-7	4	1	658	-667	
-6	4	1	1120	-1170	
-5	4	1	233	238	
-4	4	1	568	564	
-3	4	1	520	532	
-2	4	1	1397	1451	
-1	4	1	85	32	
0	4	1	1377	-1392	
1	4	1	824	-841	
2	4	1	1361	-1353	
3	4	1	845	-788	
4	4	1	1267	1206	
5	4	1	1108	1034	
6	4	1	1085	1052	
7	4	1	706	660	
8	4	1	576	-536	
9	4	1	791	-781	
10	4	1	610	-598	
11	4	1	425	-418	
12	4	1	271	276	
13	4	1	461	463	
-13	5	1	362	380	
-12	5	1	582	597	
-11	5	1	526	-533	
-10	5	1	276	285	
-9	5	1	409	-425	
-8	5	1	1153	-1189	
-7	5	1	643	628	
-6	5	1	229	246	
-5	5	1	18	5	U
-4	5	1	1844	2024	
-3	5	1	321	-333	
-2	5	1	1189	-1214	
-1	5	1	310	282	
0	5	1	1921	-2018	
1	5	1	249	-248	
2	5	1	1383	1339	
3	5	1	37	-26	U
4	5	1	1022	983	
5	5	1	864	823	
6	5	1	1304	-1282	
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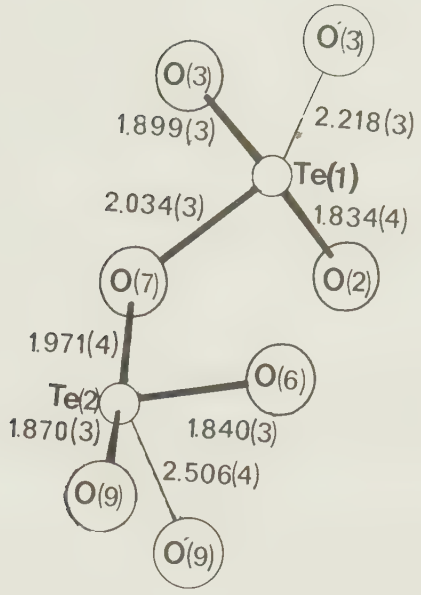

Fig. 1.

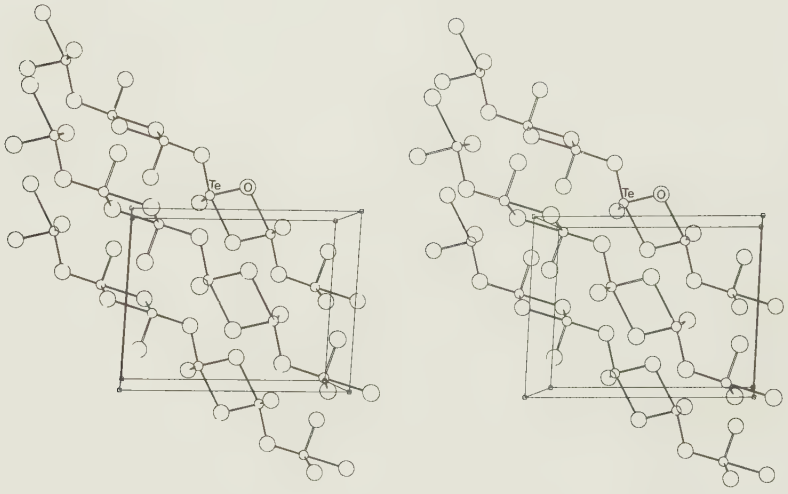

Fig. 2.

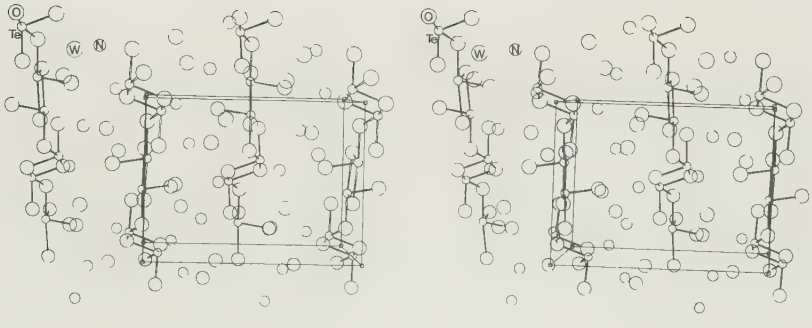

Fig. 3.

Legends to Figures

Fig. 1. The tellurium - oxygen coordination.

Fig. 2. A stereoscopic picture showing the Te - O chains, viewed along the b-axis (ORTEP; Johnson, 1965).

Fig. 3. The $(NH_4)_2Te_2O_5 \cdot 2H_2O$ structure viewed along the a-axis (ORTEP; Johnson, 1965).